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MODELLING COMPONENT REPORT FOR THE CORNWALL MISA PILOT SITE STUDY

TECHNICAL PROCEDURES FOR THE DERIVATION OF WATER QUALITY-BASED EFFLUENT LOADING LIMITS FOR POINT-SOURCE DISCHARGES TO LARGE RIVERS

(FOR INTERNAL USE ONLY)

Ontario

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TECHNICAL PROCEDURES FOR THE DERIVATION OF WATER QUALITY-BASED EFFLUENT LOADING LIMITS FOR POINT-SOURCE DISCHARGES TO LARGE RIVERS

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EXECUTIVE SUMMARY

In 1986, the Ontario Ministry of the Environment (& Energy), initiated a comprehensive pollution abatement program called the "Municipal-Industrial Strategy for Abatement (MISA)". While this program focused on the derivation of loading limits for municipal and industrial effluents based on "best available treatment - economically achievable (BATEA)", it also recognized the need to be able to derive loading limits based on the protection of water quality within the receiving water body, (i.e. "water quality-based loading limits"). In this context, "water quality" refers to the quality of not only the water itself, but also the associated sediment and aquatic-biota in the immediate vicinity of the municipal-industrial discharge(s). These "water quality-based loading limits" are sometimes derived for various classes of effluent parameters, including: conventionals, non-persistent toxics, and sometimes persistent toxics (where limitations in process and/or treatment technologies preclude their "virtual elimination").

As part of the MISA program, receiving water quality analyses were performed at six pilot sites across the province. This report summarizes the simulation modelling activities carried-out for the Cornwall MISA Pilot Site study. The main goals of this specific study were to: develop various water quality assessment techniques to quantify the relationship between effluent loading and impacts within the receiving water body; apply these techniques to establish control options for the key point source discharges; and evaluate the potential use of these techniques for other sites in the province.

The point sources considered included those of Domtar Fine Papers, Courtaulds Fibres (now closed), and the Cornwall WPCP. The Domtar diffuser discharges the effluents from Domtar, ICI (formerly CIL), Cornwall Chemicals and Stanchem. The key contaminants examined, as recommended by the Cornwall MISA Pilot Site team, were: mercury, zinc, total PCBs, benzo(a)pyrene, phenols and suspended solids.

A total of 5 mathematical simulation models were developed and applied to the portion of the St. Lawrence River into which the Cornwall point sources discharge. These models were linked to provide a direct, quantifiable relationship between the discharge of multiple point source contaminant loadings, and the resulting exposure and accumulated concentrations in the water, sediment and aquatic biota, as a function of location within the river. These models were then calibrated using existing Ontario Ministry of the Environment (MOE) field data collected between 1979 and 1991.

The multiple point source discharges considered in this study have overlapping impact zones within the St. Lawrence River. As a result, it was necessary to develop a load allocation procedure to establish loading limits. A total of 2 such procedures were devised. These procedures involve a mathematical framework, which utilizes the pertinent river condition and calibrated model factors to establish the net loading limits for each of the multiple discharges, simultaneously. The factors considered uniquely at each outfall's mixing zone, include: the upstream river contaminant background concentrations due to both the upstream river conditions and the local upstream point sources; the dispersion characteristics of the outfall's plume; and

the contaminant concentration criterion.

A stochastic load allocation procedure was developed to account for uncertainty in the load allocation results, associated with the calibration accuracy, variability in the river flow-rate, and variability in the upstream river background concentration of the contaminant. This procedure utilizes a Monte-Carlo approach, which uses quantitative information regarding the stochastic nature of the uncertainty parameters to produce multiple (stochastic) loading limits for each outfall. These multiple loading limits are then statistically analyzed to produce probabilistic loading limits. These probabilistic loading limits provide a relationship between the net contaminant loading rate and the percentage of compliance with the given contaminant criterion at the end of the mixing zone.

A very restrictive mixing zone was used for derivation of the probabilistic loading limits. Its length was set equal to the downstream edge of the "near field mixing zone". This is the zone along which the effluent plume becomes mixed over the entire water column depth. The length of this zone for the point sources considered in Cornwall ranged from about 15 to 50 metres. "Water quality based effluent loading limits", ("WQBLLs"), were developed for each contaminant and each outfall. These are taken as the most restrictive loading limit derived by considering all available environmental protection criterion concentration individually, (i.e. for impact on water, sediment and aquatic biota). The criteria used include the: "Provincial Water Quality Objectives" (PWQOs) for the water column, "Provincial Sediment Quality Guidelines" (PSQGs) - "Lowest Effect Levels" (LELs) for the bed sediment, and the "Great Lakes Water Quality Agreement" fish tissue objectives for fish in the aquatic foodweb. The recommended "WQBLLs" are based upon a 95 % compliance probability for all contaminants, except for suspended solids where a less severe 50 % compliance was chosen.

"Critical impact limits" ("CLs") were also derived for mercury, zinc and PCBs. These are taken as the probabilistic loading limits necessary to assure 95 % compliance with the PSQG - "Severe Effect Levels" (SELs). These limits are necessary to avoid severe in-place impacts, as measured in terms of contaminant concentrations within the bed sediment. As such, the "CLs" are larger than the "WQBLLs", with the difference providing an indication of the sensitivity of the benthic environment, (as measured in terms of accumulated concentrations), immediately downstream of the outfalls, to exceedences of the "WQBLLs".

The "WQBLLs" and "CLs" are provided in Table 5.6. These loading limits are compared with the measured loading rates as obtained from the various MISA monitoring programs in Table 5.7. The measured loading rate for mercury exceeded both the "WQBLL" and "CL" for all point sources. However, the total net loading of mercury from all point sources considered represented only about 2 % of the total flux passing through the St. Lawrence River. Therefore, discernable impact of mercury at the measured loading rates, would be limited to a zone along the north shore of the river, where the main portions of the plumes from the Domtar diffuser and Courtaulds shore-based outfalls pass.

Measured loadings of zinc and PCBs from the Domtar and Cornwall WPCP diffusers exceeded

their "WQBLL" values, but were well under their "CL" values. In addition, the total measured net loadings were very small when compared with the total mass flux of these chemicals passing through the St. Lawrence River. As a result, impacts of these measured loadings would only be slightly distinguishable within the near field mixing zones of these two diffusers.

The measured loadings of zinc from the Courtaulds acid diffuser and shore based outfalls greatly exceeded even their "CL" values, by about 1 and 2 orders of magnitude, respectively. As a result severe in-place impacts of zinc in the vicinity of Courtaulds would be expected, as has been measured previously by the MOEE.

The measured phenol loading from the Domtar diffuser would exceed the (95 % compliance) "WQBLL". However it would comply approximately 50 % of the time with the PWQO.

The loading of suspended solids from the Domtar and Cornwall WPCP diffusers exceeded their "WQBLL" values by about 1 order of magnitude. These measured loadings would produce mixed suspended solids concentrations at the downstream end of the mixing zone of about 2 mg/L, under the median river conditions.

The assessment techniques derived during this study were evaluated for possible use both at Cornwall (additional use) and at other provincial sites. The techniques are readily available for looking at additional contaminants at Cornwall and would likely take about a month or two to apply at another site. Hardware and software resource requirements are identified, as well as recommended staff expertise.

In addition to deriving "WQBLLs", the assessment techniques can also be used to delineate point source impact zones, evaluate hypothetical effluent contaminant loading options, and assist in the design of ambient monitoring / surveillance plans.

The main goals of this study were successfully met. Several specific conclusions were made, based upon the technical components of the work. These conclusions emphasize the importance of using a stochastic load allocation approach, which considers the effects of uncertainty introduced by model calibration accuracy and variation in river conditions, to derive loading limits for multiple point source discharges.

It is recommended that the derived "WQBLLs" be implemented where possible. These include zero net loading limits for mercury, zinc and PCBs (see Table 5.6). Other recommendations are suggested for improving the accuracy and accessibility of the assessment techniques for future applications.

This report is <u>not</u> intended to represent a new MOEE policy document. Rather, the report outlines in detail technical procedures which may be used to help establish chemical-specific "water quality-based effluent loading limits", for one (or multiple) point-source discharge(s), to large rivers, by using the Cornwall MISA Pilot Site as an example.

1. INTRODUCTION

To help protect environmentally sensitive areas within surface water-bodies, it is sometimes necessary to be able to establishment "water quality-based" effluent loading limits for conventional and non-persistent toxic chemicals on a routine basis. These limits may also be necessary for some persistent toxic chemicals, which owing to limitations of various industrial processes and treatment technologies, can not be "virtually eliminated". In all cases, the loading limits must be based upon the protection of desirable "water quality" conditions within the receiving water-body, where "water quality" includes not only the water itself, but also the associated aquatic sediment and biota that may be adversely impacted.

In 1986, the Ontario Ministry of the Environment (MOE) initiated a comprehensive pollution abatement program called the "Municipal-Industrial Strategy for Abatement (MISA)". The purpose of the program is to provide a framework for the control of toxic contaminants within industrial and municipal effluents. Much effort has been focused on development of loading limits based upon "best available technology - economically achievable" (BATEA) industrial practice and effluent treatment, via the development of effluent monitoring and limits regulations. While the development of these "technology-based" loading limits is of primary importance to the MISA program, another component of the MISA initiative focused on development of receiving "water quality-based" effluent limits to assure the protection of the aquatic environment. These "water quality-based effluent loading limits" are derived using various modelling techniques to establish predictive and quantifiable linkages between effluent loading and specific effects within the water, sediment and aquatic biota of the receiving water body in the vicinity of the outfall(s).

Receiving water quality analyses were performed at six pilot sites, chosen to represent a cross-section of municipal-industrial dischargers and receiving-water regimes in Ontario. One of these sites was the St. Lawrence River at Cornwall. This report summarizes simulation modelling activities which are intended to help meet the following goals for the Cornwall MISA Pilot Site:

i) To develop, validate and apply water quality impact assessment techniques, appropriate for the Cornwall Pilot Site area, such that a quantitative link between contaminant loading and water quality contaminant levels, can be established;

ii) To identify point source control options (if necessary) to achieve compliance with criteria designed to protect the receiving water quality; and

iii) To evaluate the potential use of the Cornwall MISA Pilot Site assessment techniques for use at other provincial sites.

The draft-final version of this report was provided to MOEE personnel in the Cornwall and Kingston offices in August, 1993. Unfortunately, the finalization of the report was unavoidably delayed due to a loss of electronic files from a retired network server. However, the various modelling techniques established and documented within the report have been used subsequently,

and are still valid and useful tools for helping to meet MOEE's environmental management needs. This report is therefore provided as a reference document for outlining technical procedures which might be used to assist in the establishment of "water quality-based effluent loading limits", for direct dischargers to large rivers (such as the Great Lakes' connecting channels). As such, the report is not intended to represent a MOEE policy document.

1.1 Point sources considered

The point sources considered in this work, are the outfalls discharging directly to the St. Lawrence River, from the following operations in Cornwall:

i) Domtar Fine Papers / ICI (formerly CIL) / Cornwall Chemicals / Stanchem; (via the Domtar diffuser),

ii) Courtaulds Fibres; (via two diffusers and the shore-based sewers), and

iii) Cornwall Water Pollution Control Plant, (via diffuser).

Although the Courtaulds Fibres has closed as of the end of 1992, it still is considered in this report for three main reasons. First of all, it was operational at the time when all field data used in calibrating the various models utilized in this study were collected. It can not therefore, be ignored in the modelling analysis performed. Secondly, deriving loading limits for the various Courtaulds' outfalls is still useful, in the event any future industrial operations resume at the site. Thirdly, the derived loading limits for Courtaulds can be used in helping to understand and explain past, present and future environmental impacts, measured or expected, in the St. Lawrence River at Cornwall.

1.2 Definition of water quality based effluent loading limits

In this work, "water quality based effluent loading limits" ("WQBLLs") for a particular point source, are the maximum allowable loadings of contaminants (at the point of discharge to the receiver), so as not to cause an unacceptable exceedence of designated contaminant concentration criteria at the end of a "regulatory mixing zone" (RMZ). The RMZ is a designated region of the receiving water body adjacent to that point source. In order to derive "water quality based effluent limits" according to this definition, in addition to a validated impact assessment technique, the following information must also be known, or defined:

i) A list of key contaminants (or surrogates), which are to be controlled at each point source;

ii) The contaminant concentration criteria necessary, for the protection of the water quality, (which includes any criteria necessary for the protection of water, sediment and aquatic biota);

iii) The location within the receiving water body, with respect to each point source and contaminant, where the criteria are to be met (i.e. the dimensions of the RMZ); and

iv) An acceptable definition of "compliance", in terms of the statistical characteristics of the key parameters involved in all aspects of the process.

As a result, this report also provides a brief description of this information as used in deriving "water quality based effluent loading limits".

It should be noted that the assessment techniques and related information used, are not exhaustive. Other appropriate methods could likely be used to obtain satisfactory results. However, due to practical resource limitations, not all methods could be tested. Therefore, the methods used were selected based upon their likely effectiveness to meet the stated needs at this Pilot Site, and thus provide a useful prototype, which may be extended or modified in future work.

2. SELECTION & DESCRIPTION OF MODELS

Different techniques are required to assess contaminant impact within the water-column, bed sediment and aquatic biota. These techniques are described in this portion of the report.

There are two main considerations in selecting the generic type of hydrodynamic and dispersion models, which are used to determine the variation of current speeds, dispersion coefficients, and contaminant concentrations within the water-column. These are whether the model should simulate steady or non-steady time conditions, and whether there should be variation in 1, 2, or 3 physical dimensions.

The time scale for significant flow rate and flow depth changes is much larger than that of the system retention time, for this short section of the St. Lawrence River (e.g. weeks as compared to hours). As a result, for a given flow rate and flow depth condition, the hydrodynamics of the system may be effectively considered as "steady" for simulation purposes.

Since the St. Lawrence River is wide, it is necessary to use a model which predicts the lateral variation in the hydrodynamics and dispersion, in addition to that in the downstream direction, (i.e. 2-dimensional). Since there is always a strong velocity gradient in the vertical dimension of large rivers, the mixing lengths required to achieve complete vertical mixing are quite short, as compared to those required for complete lateral mixing [1]. As a result, it is not necessary to model the vertical depth dimension for dispersion analysis, for most applications. However, it is necessary to know the distance downstream where the contaminant behaviour becomes well-mixed within the water-column. By definition, this location marks the transition of an effluent plume between its "near field" and "far field".

For these reasons, 2-dimensional, depth-averaged, hydrodynamic and dispersion models were

chosen to simulate contaminant concentrations within the river near the point sources. Two models were chosen, namely "KETOX", and "MSOURCE". These models have been used successfully by the MOE in examining point source impacts within the Connecting Channels of the Great Lakes in the past [3,5]. These models are similar except for the following:

- MSOURCE estimates the "near field mixing zone" dimensions for different outfall configurations and hydraulic conditions.

- MSOURCE solves the hydrodynamic and dispersion equations using a dimensional, orthogonal coordinate system (i.e. with lateral grid points measured at fixed intervals, perpendicular from the shore); whereas KETOX solves the equations at selected streamline locations, which will vary in width.

A steady-state mathematical model was developed and used to simulate contaminant impacts upon the bed sediment. This model is based largely upon mathematical equations derived by Di Toro and Paquin [6]. It is similar to the toxic substances model employed by the KETOX model, except for changes made in the derivation of the "bed layer partitioning coefficient".

In order to estimate impact upon biota within the river, two additional models were used. These are the "Thomann food chain" and "Thomann foodweb" models. These models use as input data, the simulated contaminant concentrations from the "KETOX" and "MSOURCE", in predicting impact up/within a generic aquatic food chain/food web. In addition, the food web model utilizes the predicted contaminant concentration in the bed sediment for its benthic compartment.

The details regarding the application, calibration, and sensitivity analysis, for each of these models are provided in the following sections.

2.1 The KETOX model

The KETOX model, in its current and earlier versions (known as the "KE" model), has been applied extensively with satisfactory results by the MOE to the Great Lakes Connecting Channels [2,3,4]. It is used to examine the two-dimensional (depth-averaged) dispersion and transport of discharged chemicals from multiple point sources to a Great Lakes' Connecting Channel (wide river). The mathematical theory and numerical simulation techniques incorporated by the model have been described in other MOE reports [2,3]. Thus, the following description is qualitative in nature, outlining the key features of the hydrodynamic and dispersion sub-model.

2.1.1 General Model Description

A simplified hydrodynamic model is first used to solve for the local depth-averaged velocity across closely spaced river transects (sections). The model also determines the location of the river streamlines, (which represent various accumulated percentages of total flow as measured from one side of the river). This is done at different sections along the downstream direction,

using the general Manning's equation and a shape function, which are also corrected for channel curvature effects. The model then uses a finite difference scheme to solve the stream function transformed "κ-ϵ" and mass transport equations. The "κ-ϵ" equations describe the kinetic energy of the turbulent motion and the rate of its dissipation. They are solved in order to obtain estimates of the "eddy viscosity", which are then used to indicate the values for the depth-averaged, lateral dispersion coefficients used in the contaminant transport equation [3]. This provides the concentrations of contaminant at each grid point along the selected river streamlines.

To apply the model, the river is split-up into connected "reaches" as necessary which represent the different channels of the river, as created by diversions around islands, or significant changes in the hydraulic properties of the river. It is important to have lateral profiles of the downstream velocities and river flow-rates for each of the different river reaches. These are used in calibration of the exponent used by the shape function.

KETOX uses 15 streamline-nodal points to describe the width of the river at each cross-section. Usually cross-sections are defined every 300 to 600 m for the Great Lakes' Connecting Channels. This is done for each channel of the river.

The required input data for this submodel includes: the total flow rate in the river channel; flow depths and widths at the selected cross-sections under the given river channel flow rate; initial depth-averaged current speed and background chemical concentrations across the upstream end of the river channel (i.e. where the simulation begins) ; locations of all outfalls and their associated contaminant loading rates; and the total loss rate (due to volatilization or transformation) of the chemical within the water-column of the river channel. The river bed "roughness" and energy slope of the river are implicitly provided by describing these input data, and thus do not need to be explicitly given to the model.

These input and output data, are specific to the given steady state river flow, and outfall loading conditions. Thus, the variation of these input data due to changes in either river flow, or loading conditions, must also be known, if these are to be simulated.

2.1.2 Input Data

2.1.2.1 Hydrodynamic data and discretization:

The section of the St. Lawrence River simulated by the KETOX model, is about 13 km long, stretching approximately from the West-end of Cornwall Island downstream to the east-end of St. Regis Island, as shown in Figures 2.1 and 2.2. This section receives the discharges from all outfalls considered by the Cornwall MISA Pilot Site study.

The selection of reaches for the KETOX model was dictated by the general river flow configuration in the simulated section of the river. A separate reach, was used to represent each channel of the river, as formed by the various islands. These reaches are shown in Figure 2.2.

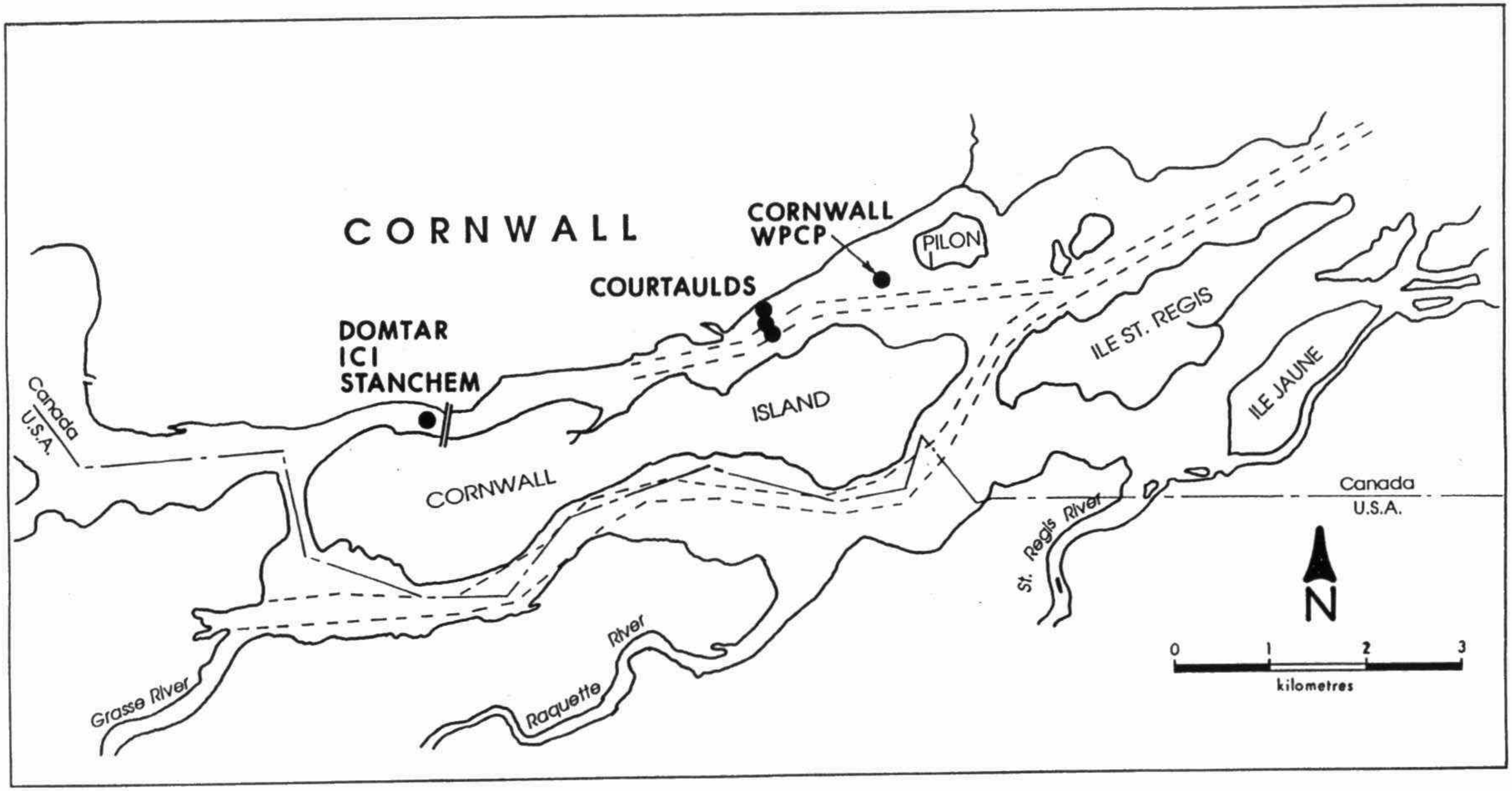


FIGURE 2.1: Study area for the Cornwall MISA Pilot Site

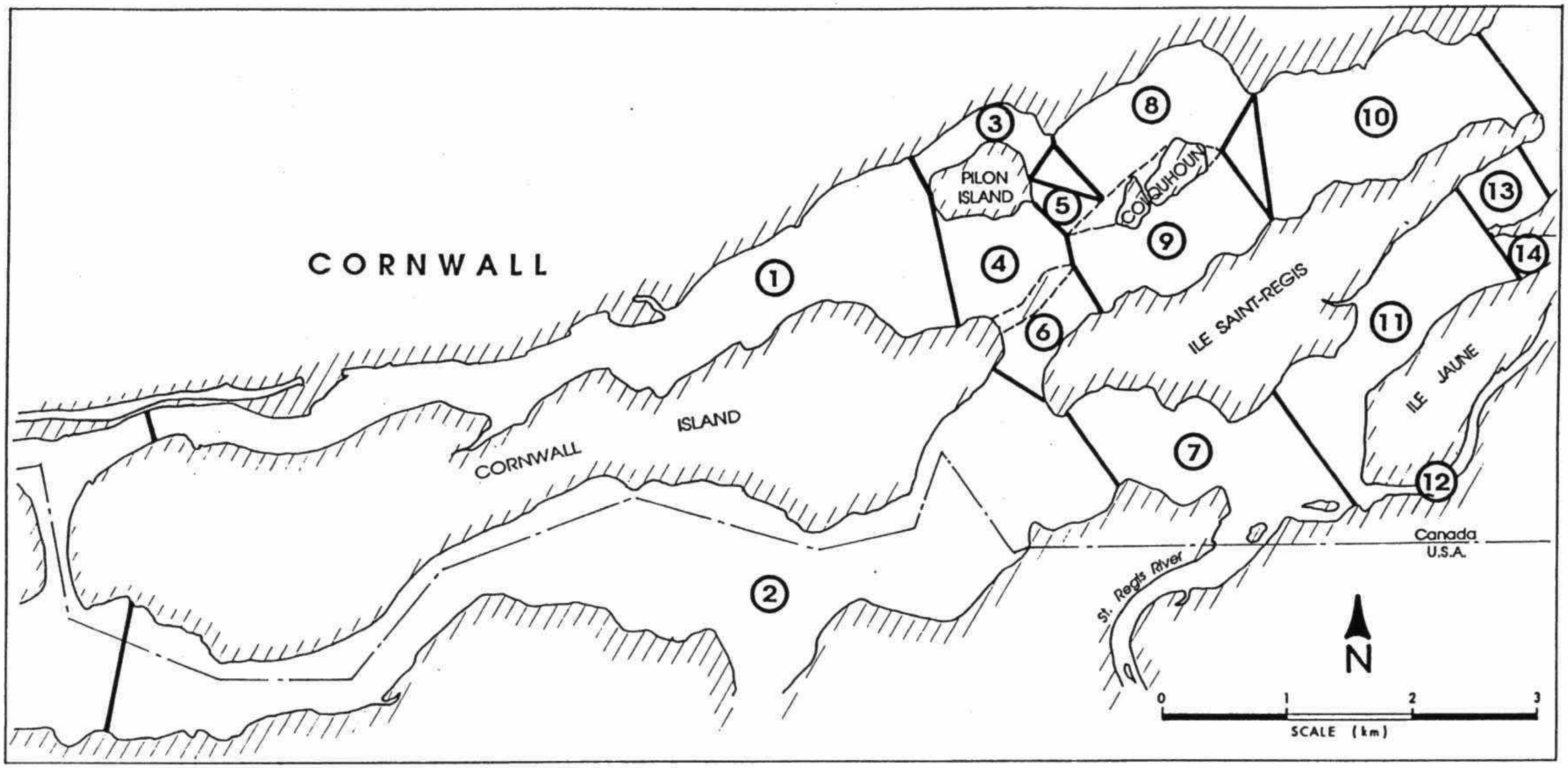


FIGURE 2.2: River reaches for the "KETOX" model

The cross-sections within each KETOX reach, were set at every 1000 feet, as shown in Figure 2.3. The depths at 40 equally spaced distances across each cross-section, were estimated using Canadian Hydrographic Service Charts No. 1413 and 1414.

Three river flow conditions were considered, namely the: maximum, average, and minimum, mean-monthly flow rates, as released through the Moses-Saunders Power Dam, between 1960 and 1980 [7]. The values for these three flow-rates are respectively about: 9,900, 7,200, and 5,000 cms. The river stages (levels) associated with these three flow rates are estimated to be: +0.70, +0.43, and -0.30 m [8]; above those indicated on the Navigational Charts which are based upon the 1955 International Great Lakes Datum.

The percentages of the total river flow rate passing through each of the channels in the Cornwall vicinity, are summarized in Figure 2.4. These are based upon field measurements taken by the MOE during 1988 [9].

2.1.2.2 Sources and Contaminant Loading estimates:

A total of 5 diffusers/outfalls were identified for purposes of the Cornwall MISA Pilot Site study. These are namely the:

i) Domtar / C.I.L. / Cornwall Chemicals common diffuser,
ii) Courtaulds, viscose / sulphide diffuser,
iii) Courtaulds, acid diffuser,
iv) Courtaulds, shore-based outfall, and
v) Cornwall, Water Pollution Control Plant diffuser.

The Courtaulds shore-based outfall actually represents 4 separate sewers, namely: combined storm, acid recovery, tank car unloading and Caravelle carpets. They are located relatively close together, and discharge to a nearshore region which has relatively low flow velocities. Therefore for modelling purposes, they are treated as a combined single outfall. This combined outfall is referred to as the "Courtaulds shore-based outfall" or point source, in the remainder of this report.

The key characteristics of these diffusers / outfalls, in terms of modelling the impact of their discharged effluent upon the river, are provided in Table 2.1.

A total of 5 parameters of concern were identified by the Cornwall MISA team, for purposes of modelling. These include:

i) Mercury (Hg),
ii) Zinc (Zn),
iii) total Polychlorinated Biphenyls (PCBs),
iv) Benzo (a) pyrene (BAP), and
v) Phenol.

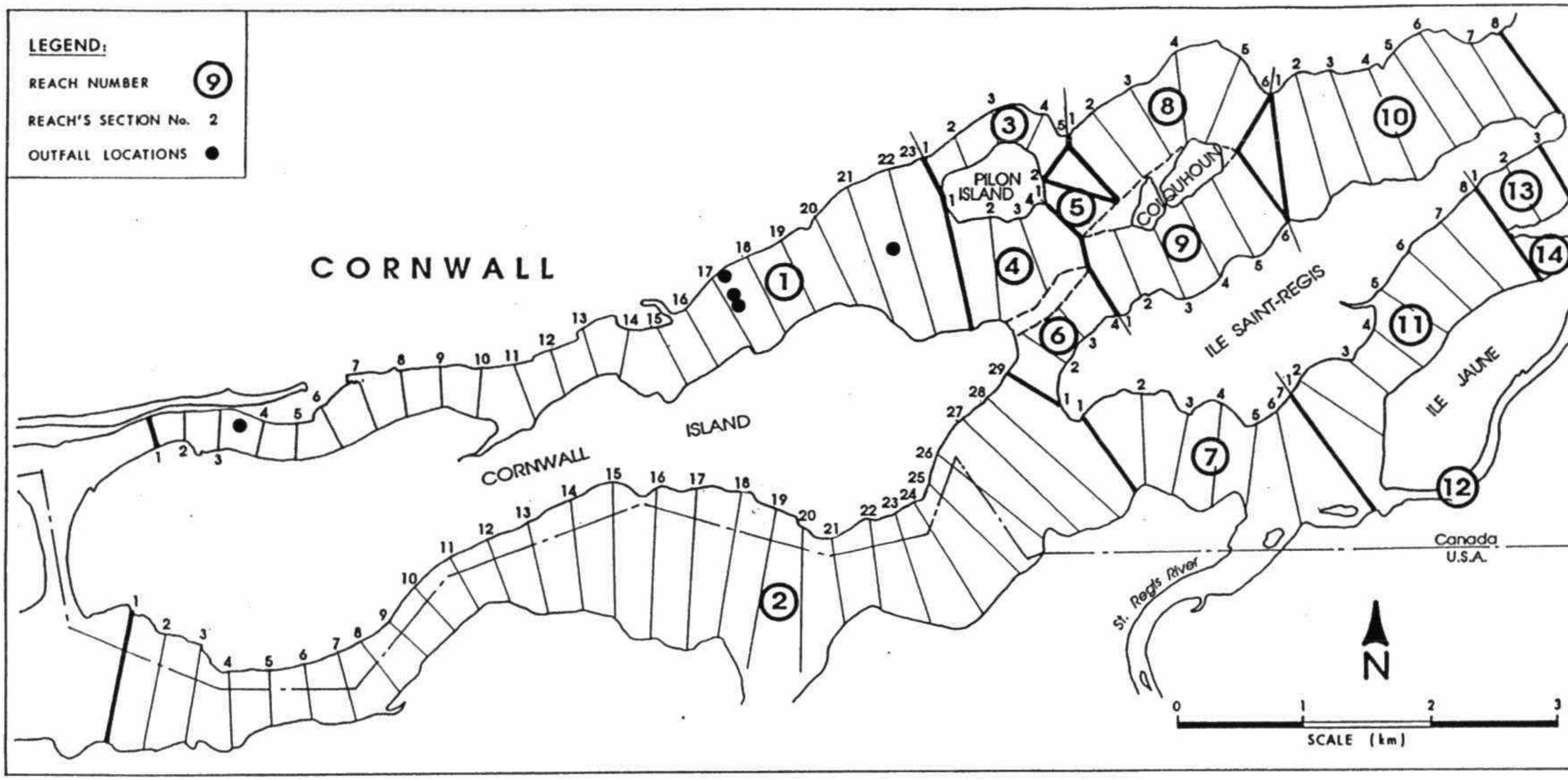


FIGURE 2.3: River cross-sections for the "KETOX" model

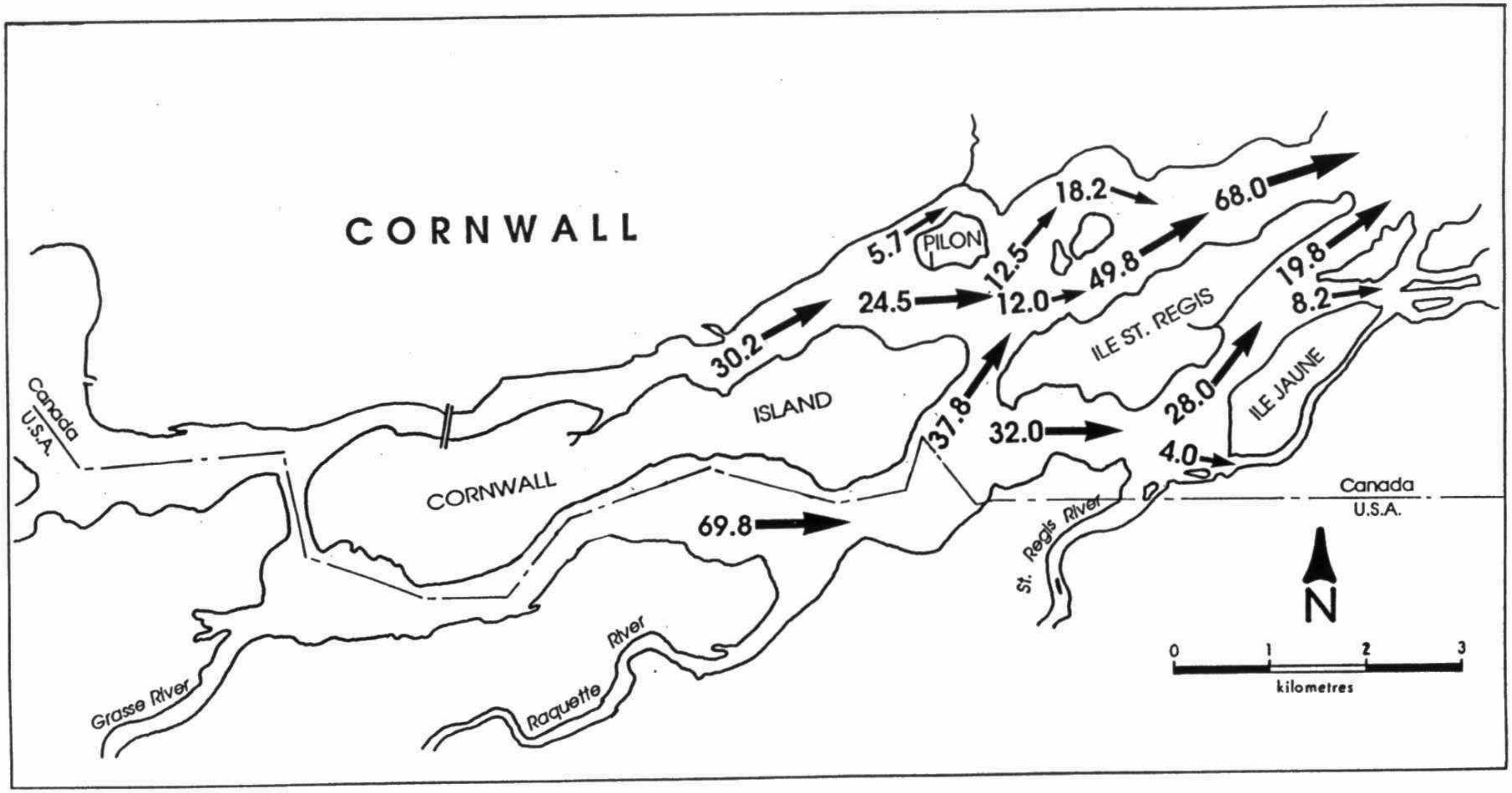


FIGURE 2.4: Distribution of total river flow

Table 2.1 Characteristics of the Cornwall MISA point sources.

POINT SOURCE	Approx. Distance Shore to Discharge [m]	Discharge Dimensions		Effluent Flow Rates [m ^ 3/sec]	
		Diffuser Length [m]	Outfall Area [m ^ 2]	Measured Ranges	Value Used
Domtar/CIL/ Cornwall Chem. Diffuser	63	48	0.5	1.39 – 1.69	1.53
Courtaulds – Viscose/Sulphide Diffuser	230	12	0.14	0.018 – 0.107	0.107
Courtaulds – Acid Diffuser	212	12	0.14	0.042 – 0.082	0.082
Courtaulds – Comb'd Storm Outfall	15	–	1.1	0.029 – 0.117	0.063
Cornwall WPCP Diffuser	602	15	0.4	0.44 – 0.77	0.564

Note: These data are based on References 10, 27, 28, 29 and 30.

Suspended solids were also considered in order to examine the differing transport and fate characteristics of both the "dissolved" and "adsorbed" phases of the parameters of concern.

The estimated range of loading rates of the parameters of concern, from all point sources, are listed in Table 2.2. These rates are based upon measured "whole-water" concentrations within the effluents and measured or estimated effluent flow rates. The measurements were taken via separate studies carried-out between 1979 and 1988, [10,11,12,13,14]. The calibrations of the models are based upon these data bases.

Three types of parameter loading information is provided for each of the 5 point sources in Table 2.2. These include the gross range, the average due to river background, and the net range. The gross loading range is based upon the actual measured parameter concentrations and effluent flow rates. The average loading due to river background represents that which is expected in the effluent if no chemical loading is added to the effluent by the plants, (i.e. it is contained within an equivalent quantity of background river water). The net loading range is obtained by subtracting the loading due to river background, from the gross measured loading. Also for comparison purposes, the average concentrations and "mass fluxes" of background chemicals, contained within the water passing through the river channel north of Cornwall Island, are provided in Table 2.2.

In 1988, the effluents of four of the point sources (not including the Courtaulds shore-based sewers), were centrifuged, and the suspended solids obtained analyzed for adsorbed contaminants by the MOE [14]. Using measured suspended solids concentrations, and estimated effluent flow rates, loadings of the parameters of concern adsorbed onto discharged suspended solids were calculated. These results are listed in Table 2.3. Also provided in this table are the total loading rate of the parameters of concern (i.e. within the "whole-water") discharged from the point sources. The calculated ratio of "particulate" to "whole-water" loading is also provided. Generally, this ratio tends to increase when considering Zn, Hg, and Benzo (a)pyrene, respectively, (total PCBs were not detected). The ratio for Zn, and Hg, are significantly different within the Courtaulds Acid Diffuser effluent, as compared with the other effluents.

Table 2.3 also provides similar information for centrifuged suspended solids collected at 5 MOE stations in the river itself. These locations are provided in Figure 2.5.

2.1.3 Model Calibration

The hydrodynamic model is calibrated by adjusting an exponent used by the shape function. Within each river reach, at the cross sections where velocity measurements have been taken, the shape function is used to adjust the "shape" of the depth-averaged velocity profile across the reach, in order to match the measured velocity profile. A calibrated shape function exponent was obtained for each reach of the river, using the current meter data collected by the MOE in 1988 [9]. The calibrated values and comparison of predicted and measured depth-averaged current velocities, are provided in Figures 2.6 (a) through (f).

Table 2.2 **Estimated GROSS and NET loading rates from the point sources, during the 1979–1988 time period.**
(Based on data from Reference 10)

SOURCE (Assumed flow rate, in m^3/sec)	Type of Load	PARAMETER LOADING RATE (kg/day) Suspended solids	Hg	Zn	Total PCBs	Benzo(a)pyrene	Phenol
River Background Concentration Used: [in ug/L]	–	900	0.15	7	0.0012	–	0.0011
Background Mass Flux, passing via: – entire river (7200)	RB	559800	93.5	4360	0.72	–	0.677
– Cornwall Channel (2180)	RB	169500	28.3	1320	0.218	–	0.205
Domtar/CIL/ Cornwall Chem. Diffuser (1.54)	G	7800 – 16800	.070 – .252	8.7 – 19.2	.017 – .060	.012	18.7
	B	120	0.02	0.93	0.00015	–	0.00014
	N	7700 – 16700	.050 – .232	7.8 – 18.3	.017 – .060	–	18.7
Courtaulds – Viscose/Sulphide Diffuser (.055)	G	186 – 2781	.0039 – .0182	4.3 – 32.7	.00096	ND	ND
	B	4.3	0.0016	0.03	6.0 x 10^–6	–	5.14 x 10^–6
	N	182 – 2780	.0023 – .0166	4.3 – 32.7	.00095	–	–
Courtaulds – Acid Diffuser (.042)	G	208 – 411	.0041 – .0087	22 – 359	.00039	ND	ND
	B	3.3	0.0012	0.03	4.0000000E–06	–	4.0 x 10^–6
	N	205 – 408	.0029 – .0075	22 – 359	.00039	–	–
Courtaulds – Storm Outfall (.029)	G	13 – 457	.00065	.34 – 2.94	ND	ND	ND
	B	2.3	0.00083	0.02	3.0 x 10^–6	–	2.72 x 10^–6
	N	11 – 455	0	.32 – 2.92	–	–	–
Cornwall WPCP Diffuser (0.58)	G	1060 – 3230	.00042 – .00260	1.34 – 4.95	.0025 – .0088	ND	.093 – .318
	B	45	0.00746	0.35	5.8 x 10^–5	–	5.42 x 10^–5
	N	1020 – 3190	0	.99 – 4.60	.0024 – .0087	–	.092 – .317

Legend:
RB = mass flux passing by within the river, due to the general upstream background concentration
G = GROSS loading from point source
B = loading due to the general river background concentration (ie. passed through the plant)
N = NET loading from the point source, (ie. N = G – B)

Table 2.3 Estimated total and particulate concentrations and loads.
(Based on data from Reference 14)

Location	Suspended Solids Conc. (mg/L)	Assumed Outfall Flow-rate (m^3/sec)	Parameter	Particulate concentrations and particulate / total loadings.			
				Hg	Zn	Total PCBs	Benzo(a) pyrene
I. OUTFALLS:							
Domtar/CIL/	112	1.54	C'p	1.4	138	ND	0.72
Cornwall Chem.			Lp	0.021	2.1		0.011
Diffuser			Lt	0.082	15.4	ND	0.012
			Lp/Lt	0.26	0.14		0.92
Courtaulds –	49.6	0.0547	C'p	3.50 [1]	3140 [1]		0.058 [1]
Viscose/Sulphide			Lp	0.00088	0.79		1.45x10^-5
Diffuser			Lt	0.00385	4.33	ND	
			Lp/Lt	0.23	0.18		
Courtaulds –	90.7	0.0425	C'p	48.5	5100		0.265
Acid Diffuser			Lp	0.0161	1.7		8.8x10-5
			Lt	0.0041	178	ND	
			Lp/Lt	3.93	0.01		
Cornwall	21.3	0.575	C'p	1.35	130	ND	0.52
WPCP Diffuser			Lp	0.0014	0.14		55.x10^-5
			Lt	0.0042	1.34	ND	ND
			Lp/Lt	0.33	0.1		
II. RIVER STATIONS:							
MOE 401 / EC 12	2	–	C'p	0.15	150		0.09
			Cp	0.0003	0.3		0.00018
			Ct	0.01	12.8	0.0007	0.00011
			Cp/Ct	0.03	0.023		1.64
MOE 402 / EC 4	2	–	C'p	0.15	150		0.13
			Cp	0.0003	0.3		0.00026
			Ct	0.01	6	0.002	0.00021
			Cp/Ct	0.03	0.05		1.24
MOE 69 / EC 2	2	–	C'p	0.16	150		0.08
			Cp	0.00032	0.3		0.00016
			Ct	0.06	4.2	0.002	
			Cp/Ct	0.005	0.071		
MOE 74 / EC 9	2	–	C'p	0.18	190	0.13	0.13
			Cp	0.00036	0.38	0.00026	0.00026
			Ct	ND	19.5	0.001	
			Cp/Ct		0.019	0.26	
MOE 372 / EC 8	2	–	C'p	0.22	155		0.65
			Cp	0.00044	0.31		0.0013
			Ct	0.005	11.1	0.002	0.0003
			Cp/Ct	0.088	0.028		4.33

PARAMETER DEFINITIONS:

C'p = Measured PARTICULATE chemical concentration, (mg/kg).
Cp = Calculated PARTICULATE chemical concentration in whole water, (ug/L).
Ct = Measured TOTAL chemical concentration in whole water, (ug/L).
Lp = Calculated chemical loading associated with PARTICULATE material, (kg/day).
Lt = Calculated chemical loading, TOTAL (ie. in whole water), (kg/day).

[1] = These are weighted averages of the individual values from the Viscose and Sulphide Sewers.

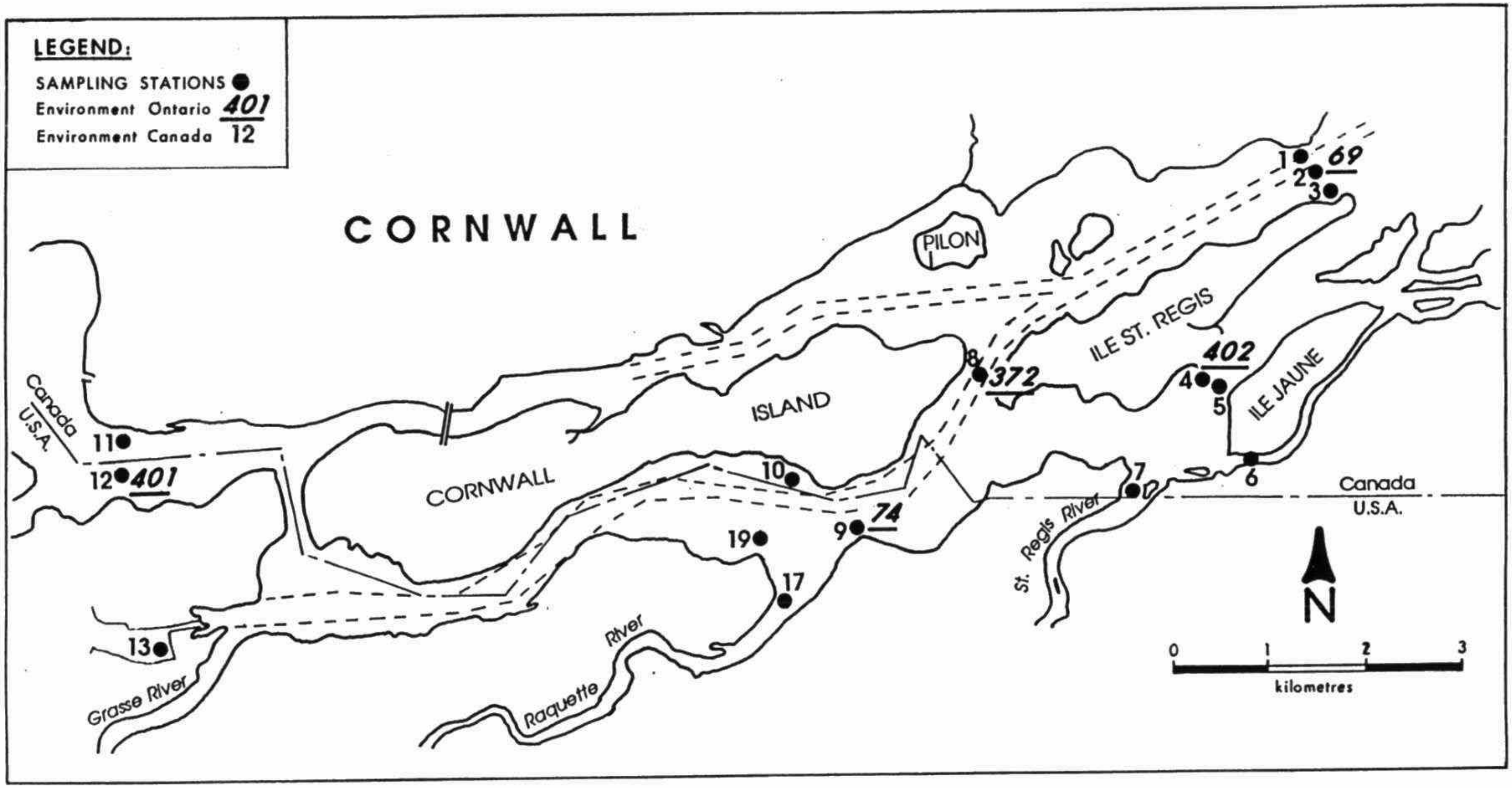


FIGURE 2.5: River stations for the 1988 Suspended solids study (Reference 14)

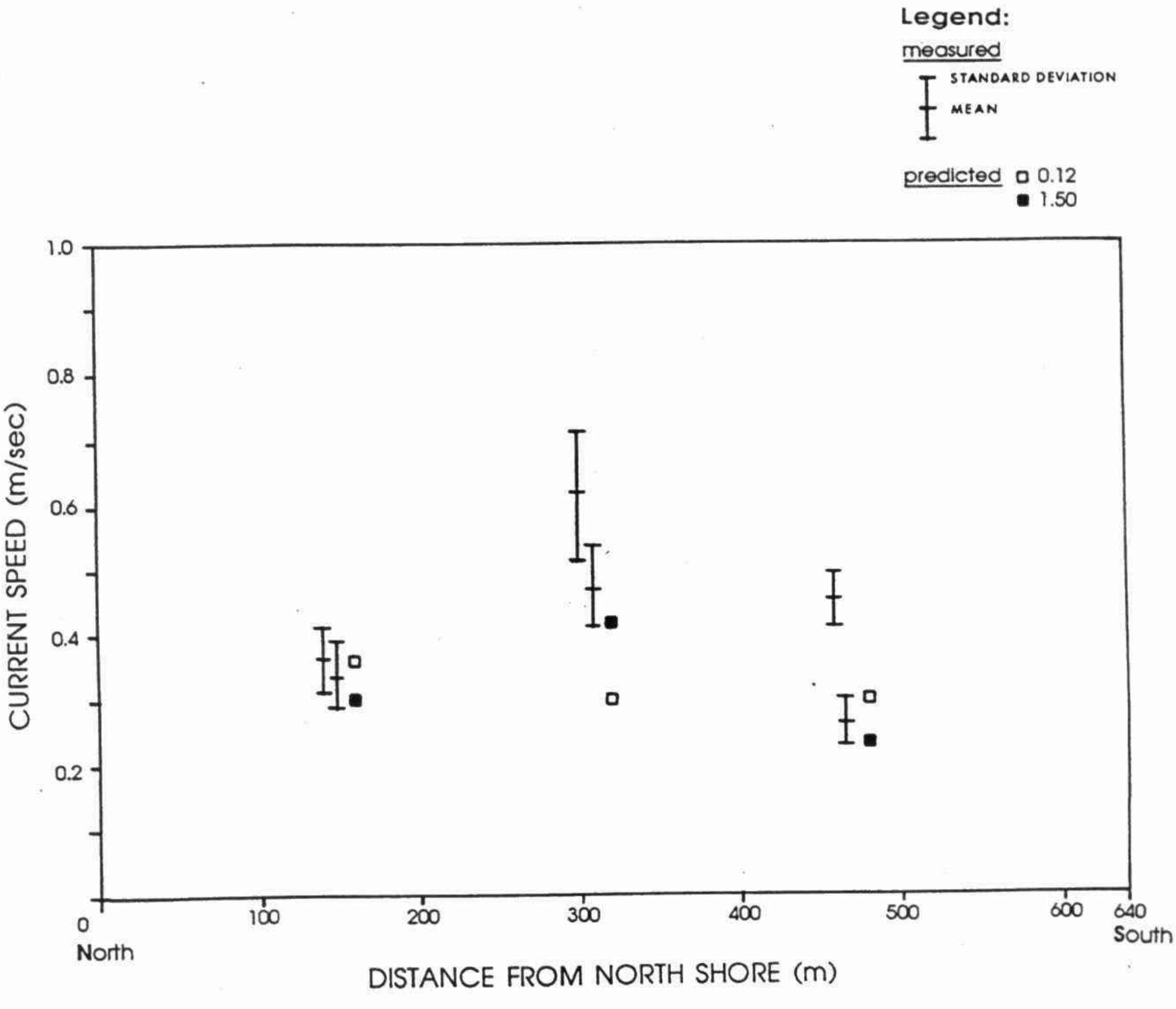


FIGURE 2.6a: Predicted vs. Measured depth-averaged current velocities near "KETOX: Reach 1 - Cross Section 19"

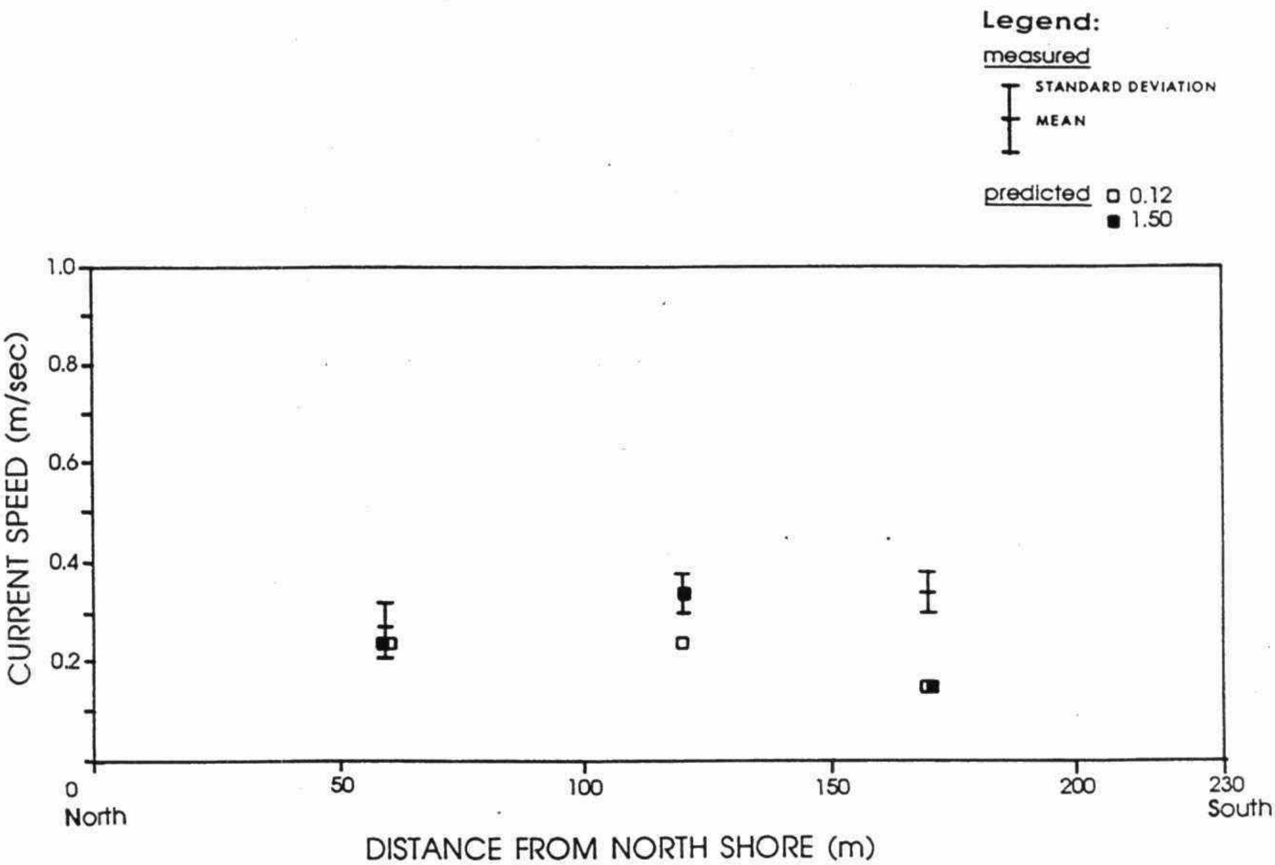


FIGURE 2.6b: Predicted vs. Measured depth-averaged current velocities near "KETOX: Reach 3 - Cross Section 2"

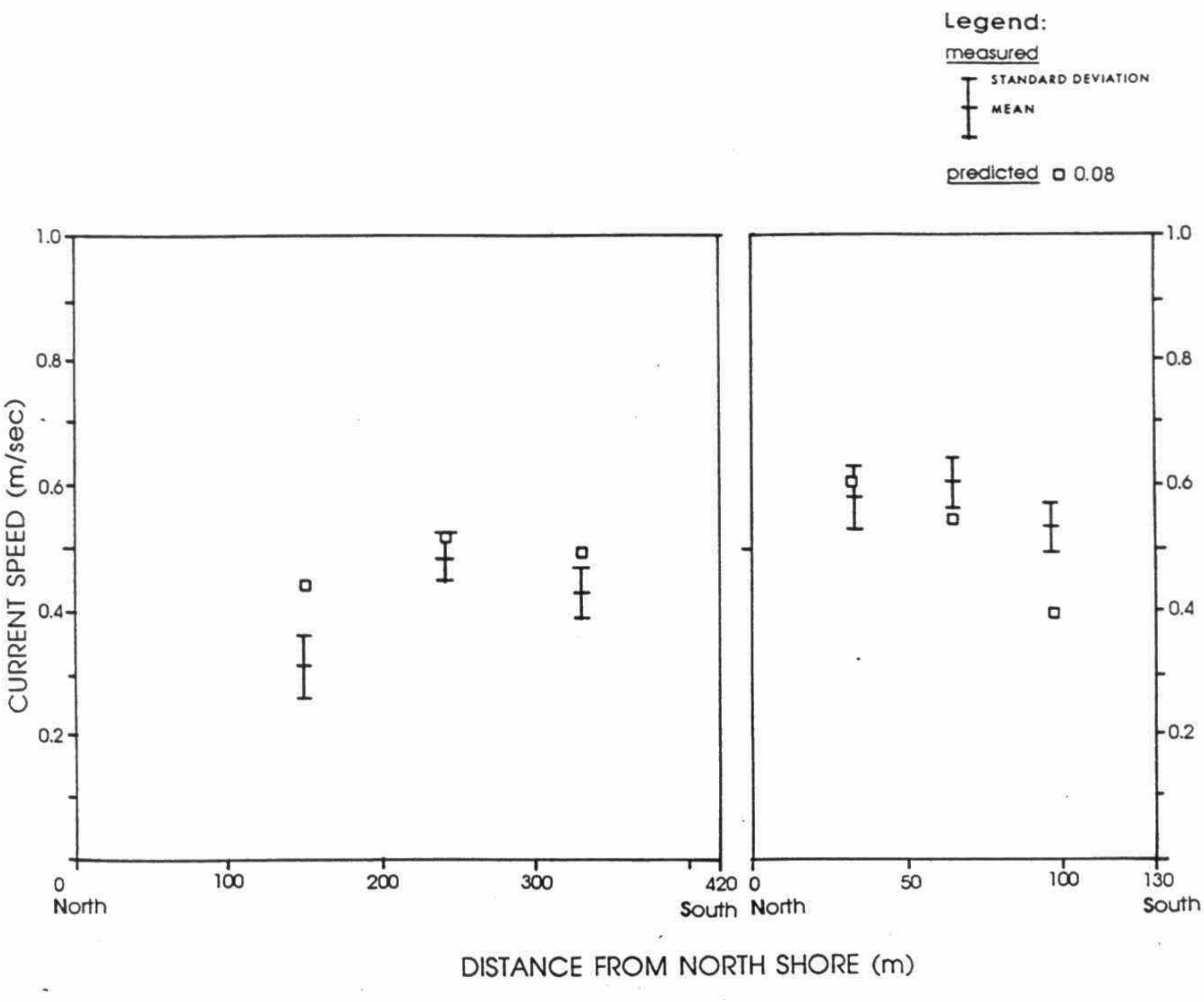


FIGURE 2.6c: Predicted vs. Measured depth-averaged current velocities near "KETOX: Reach 4 - Cross Section 4"

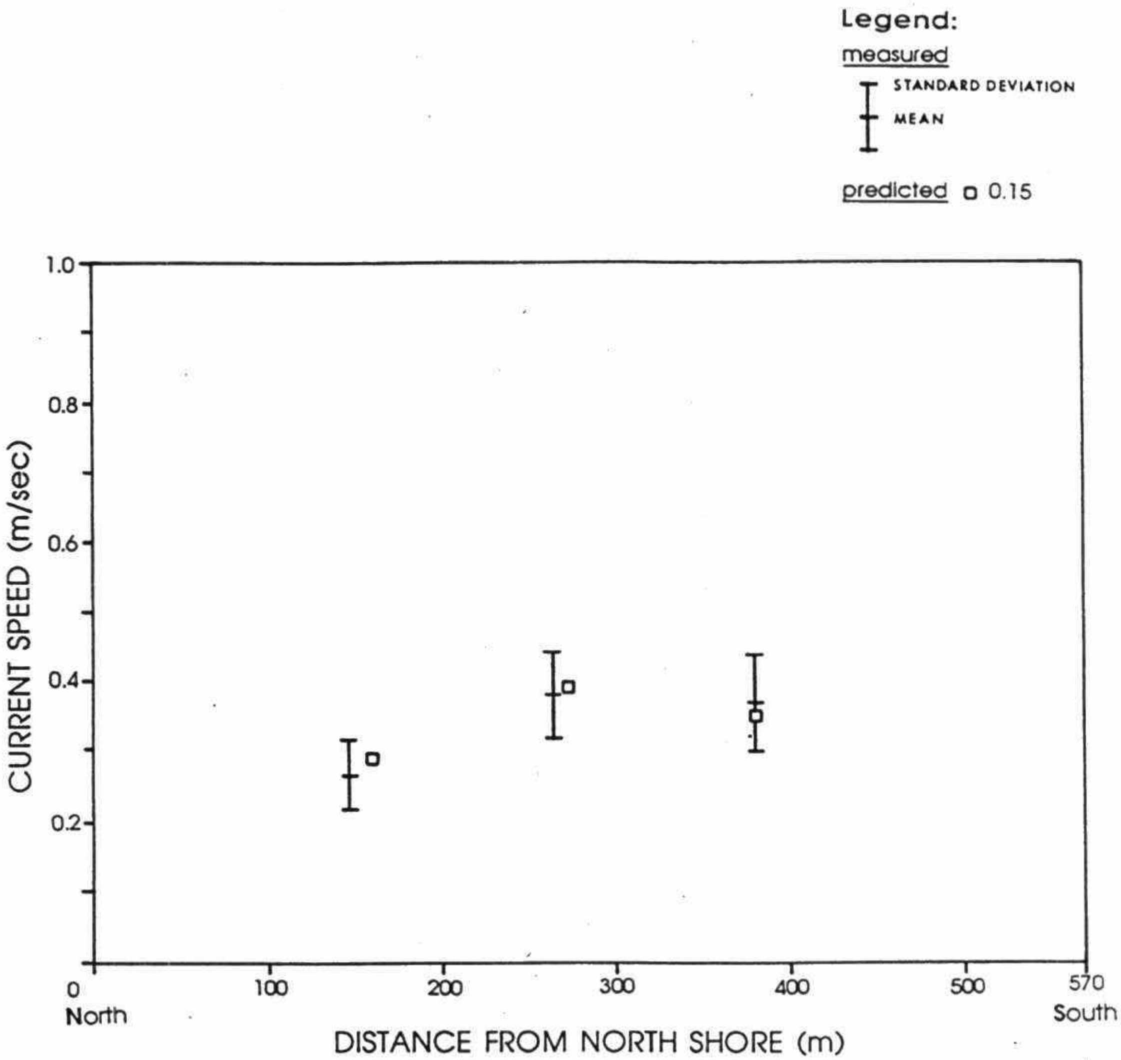


FIGURE 2.6d: Predicted vs. Measured depth-averaged current velocities near "KETOX: Reach 8 - Cross Section 4"

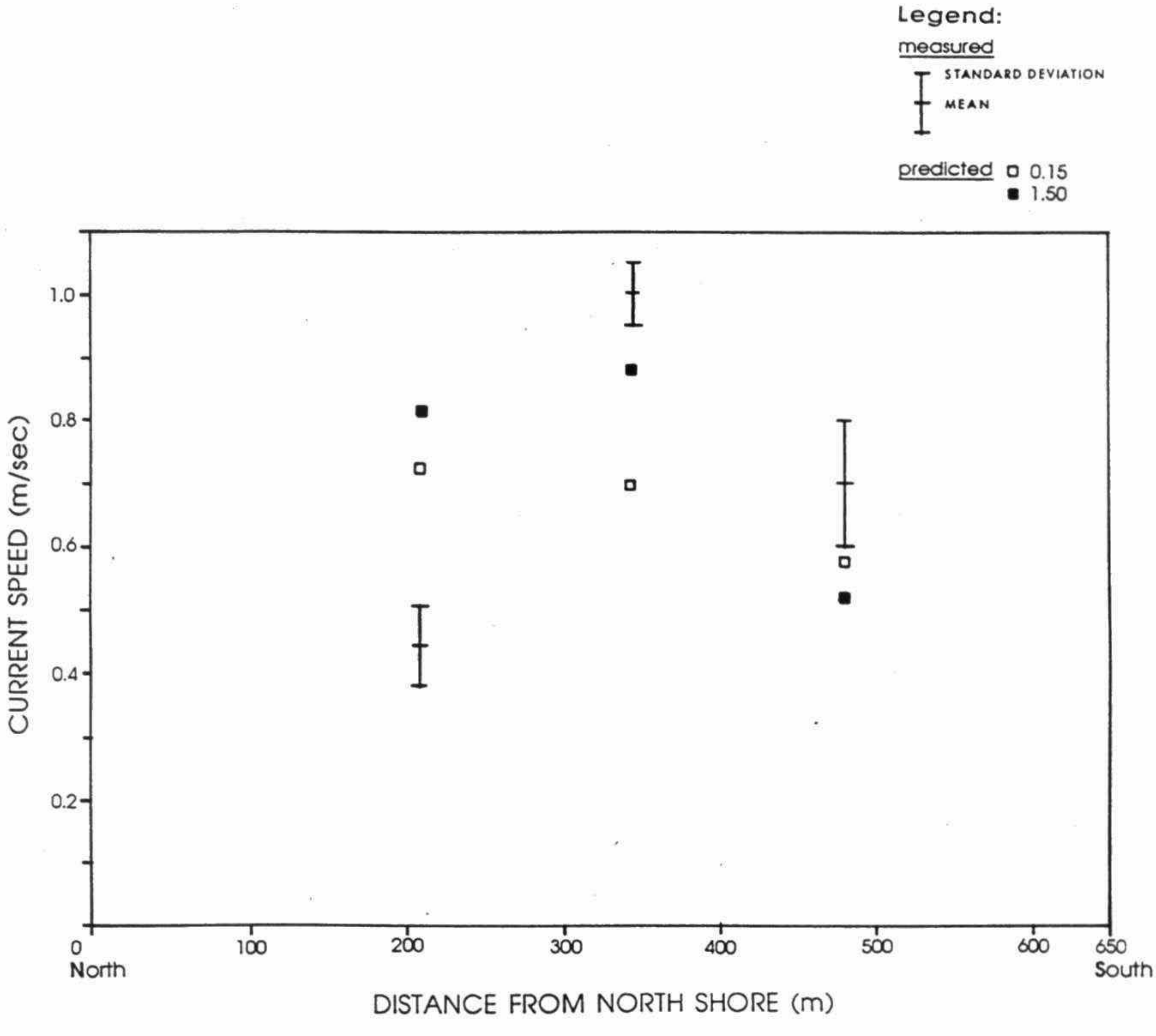


FIGURE 2.6e: Predicted vs. Measured depth-averaged current velocities near "KETOX: Reach 9 - Cross Section 6"

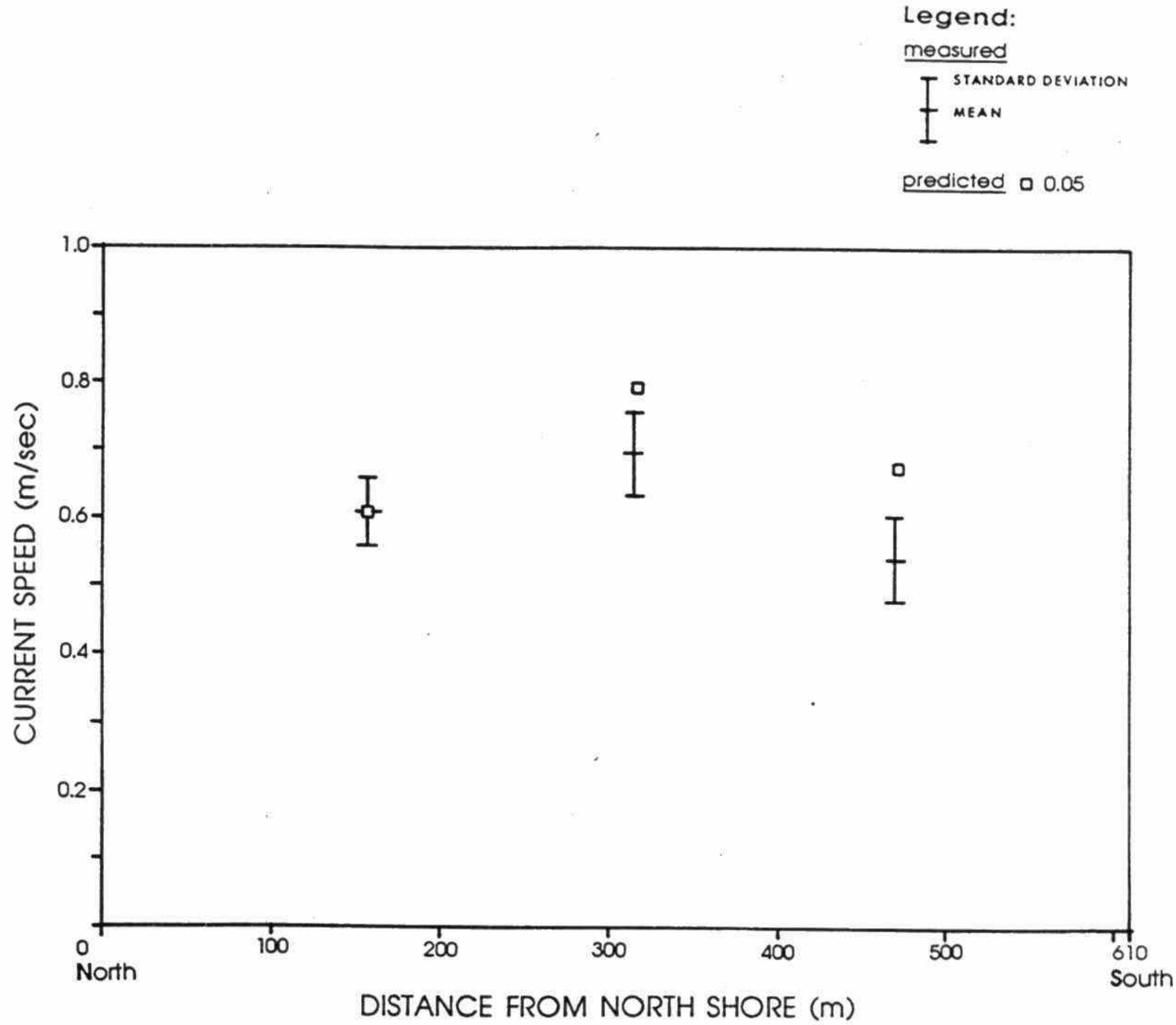


FIGURE 2.6f: Predicted vs. Measured depth-averaged current velocities near "KETOX: Reach 10 - Cross Section 8"

The "κ-ϵ" subroutine of the program, estimates the value of the depth-averaged lateral dispersion coefficient, at each node where the equations are solved. This coefficient is the major factor influencing the dispersion of contaminants discharged at a steady rate within an effluent, as they travel downstream from the outfall. The model also provides a factor by which all calculated dispersion coefficients within each river reach can be adjusted.

The total phenolics data set collected during July, September, and October of 1980 by the MOE [10], was used to provide the loading and river concentration data required for the dispersion calibration. This parameter was chosen because it provided the most comprehensive information for calibration. Although the total phenolics measurements consist of several isomers, it is likely that these will effectively behave conservatively within the geographical region used for the calibration. Further, in selecting a parameter for dispersion calibration, it is necessary that the ratio of point source loading to river background loading, be large enough so as the impact within the river caused by the point source, is clearly discernable. This is the case for total phenolics, but is not the case for most of the conventional and metal parameters.

Phenolics data were collected at 18 river stations, located as shown in Figure 2.7. A total of 14 or 15 measurements were made at each of these stations. The total phenolics loadings were estimated [10] to be about 116 and 0.64 kg/day, from the Domtar / CIL / Cornwall Chemicals, and Cornwall WPCP Diffusers, respectively, during 1980. This was based upon between 12 and 15 effluent samples.

Using these data, the model was run using various values for the lateral dispersion adjustment factor, until the best fit of measured and predicted data was found. The stations of most importance were the transects of Stations 61, 62 and 63. For calibration purposes, the optimum value of the dispersion adjustment factor will predict similar concentration ratios for the stations along each transect. The comparison between predicted and measured concentrations is shown in Figure 2.8. The average background concentration of total phenolics (i.e. upstream of the Domtar / CIL / Cornwall Chemical Diffuser), during the time of these measurements was estimated to be about 0.3 ppb, and is incorporated into this calibration analysis.

The best value found for the lateral dispersion adjustment factor, was about 0.33. Using this value, and the estimated 0.3 ppb background concentration, the average absolute error (with respect to the measured concentrations) for the 16 stations was only about 21 %.

2.2 The MULTISOURCE model

The MULTISOURCE model, was originally developed and applied to the St. Lawrence River at Cornwall via an MOE contract [5]. It is similar to the hydrodynamic / dispersion portion of the KETOX model. It is used to determine the two-dimensional (depth-averaged) dispersion and transport of discharged chemicals to the water-column of a wide river. The mathematical theory and numerical simulation techniques used by the MULTISOURCE model are best described in two publications, [5,15]. Since it is quite similar to the KETOX model, only the important differences used in this study are outlined in Sections 2.2.1 through 2.2.3.

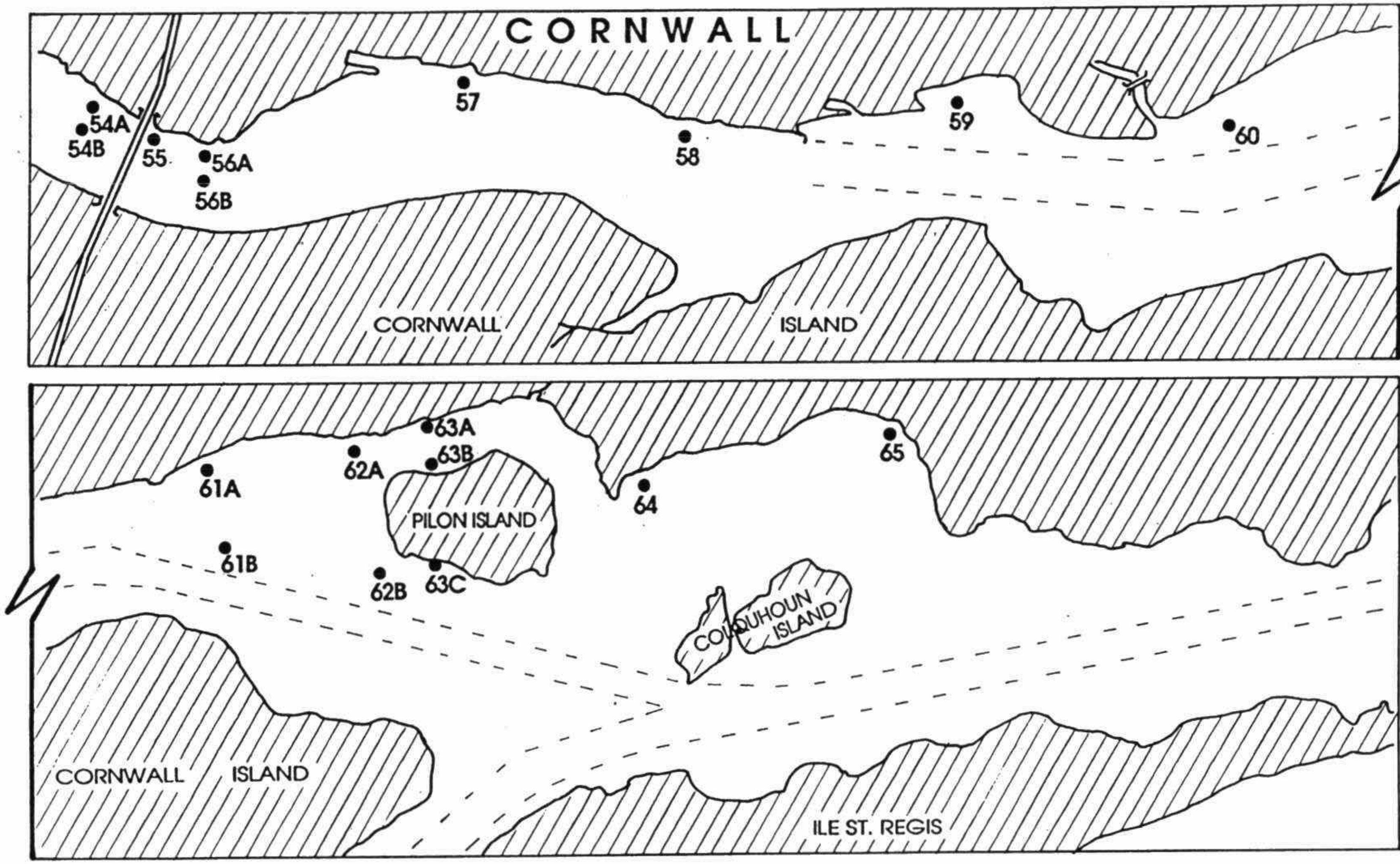


FIGURE 2.7: Stations where phenolics were measured. (Reference 10)

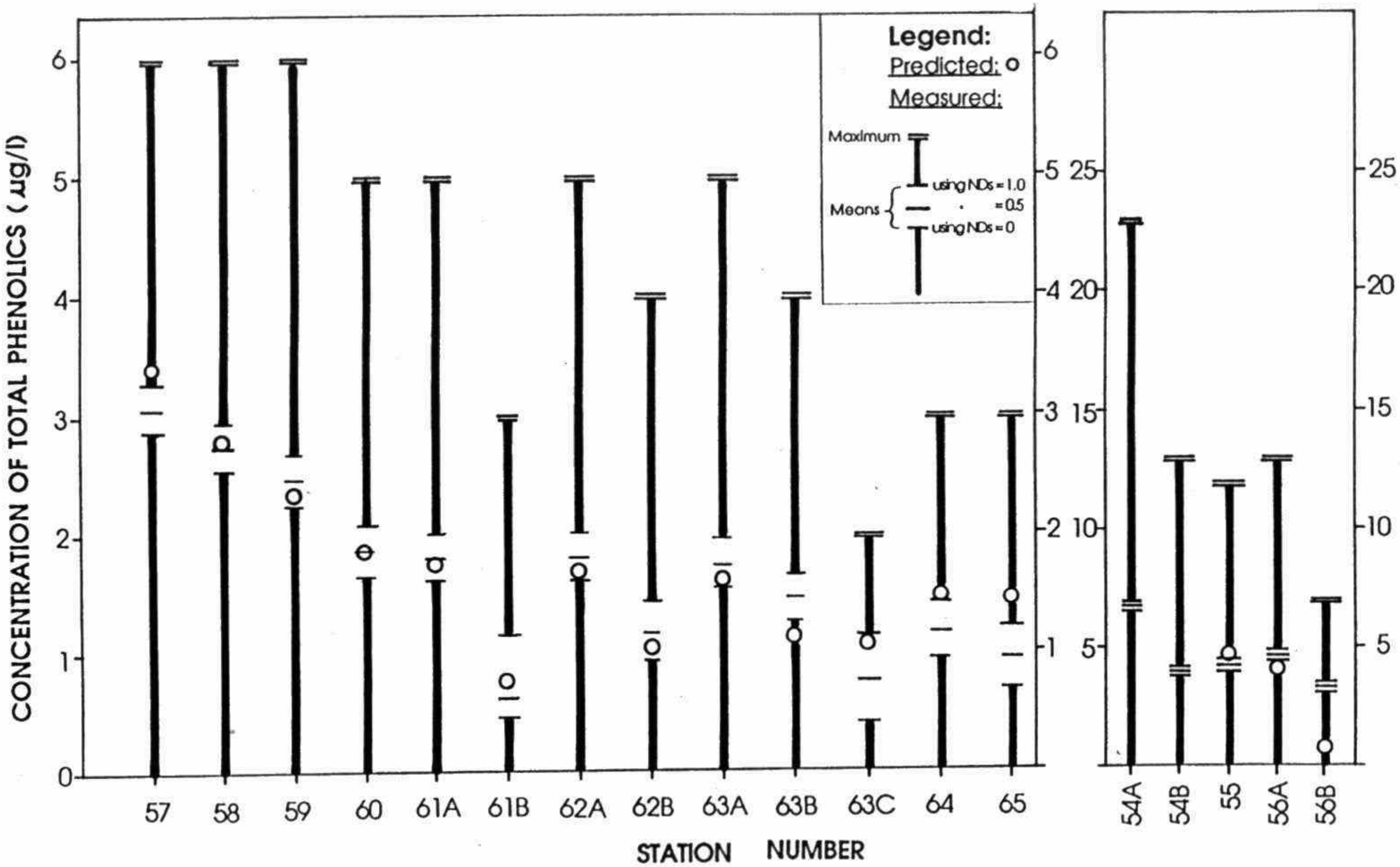


FIGURE 2.8: Predicted vs. Measured phenolics concentrations.

2.2.1 General Model Description

The MULTISOURCE model is as described in Section 2.1.1, except for the following:

i) It does not solve for the location of the flow streamlines.

ii) No stream function transformation of the basic equations is used.

iii) The model solves for the depth-averaged concentrations of contaminant, at grid points with fixed lateral and longitudinal spacings, set by the user.

iv) The model can only be applied to one reach at a time, (i.e. there are no river flow "split" and "combine" options).

v) The exponent for the lateral profile of depth-averaged velocities is fixed at a value of 1/6, with Manning's Coefficient set as a variable input parameter.

vi) The model reads in river depths at fixed width intervals, for all river sections, (e.g. usually set at every 100 ft).

vii) The model incorporates a subroutine which calculates the dimensions (i.e. plume width and downstream distance), of plumes at the end of the near field mixing zone (i.e. where the plumes have been assumed to cover the entire vertical water-column depth of the river). Options exist for estimating these data for various types of outfalls and diffusers. The calculated near field plume properties, are then used as input to the far field dispersion and transport simulation portion of the model.

This model (via features iii and vii above), is better suited to look at detailed water-column impact in the immediate downstream vicinity of outfalls. This is outlined in greater detail later on.

2.2.2 Input Data

The description of these data are similar to those outlined in Section 2.1.2.

The depths used by the model were taken at intervals of 100 ft along river transects located about 1000 ft apart.

2.2.3 Model Calibration

The version of the MULTISOURCE model used in the current study, requires that two key parameters be calibrated. These include Manning's coefficient, (used in the flow hydrodynamics), and a dimensionless dispersion factor. This dimensionless dispersion factor is used to adjust the calculated value of the dispersion coefficient, (which is based upon the local

shear velocity and flow depth [5]).

The MULTISOURCE model was used previously, to examine the impact of 6 selected parameters upon the Cornwall Channel (i.e. the portion of the St. Lawrence river north of Cornwall Island) [5]. This was done for 5 point sources, including three of the four diffusers considered in the current study. As part of this previous application, the model was calibrated, tested, and deemed to perform satisfactory. The values used in this previous work include a Manning's coefficient of 0.0235, and a dispersion factor of between 0.96 and 2.0.

These values were used in the present study. Using either extreme value of the dispersion factor, did not significantly change the predicted concentrations, in the river locations represented by the 1980 calibration stations. A dispersion factor of 0.96 was used to obtain the predicted results which are compared to those measured in Table 2.4. The resulting average absolute error in the predicted concentrations, with respect to those measured at Stations 55 through 61 A, is about 36 %. It appears that some of this error is caused by inaccurate estimation of the locations of the stations, (which were not accurately measured). This is important to this model due to its fine resolution. By comparing the maximum predicted concentrations at each river section where the stations were located to the same station data, the resulting average absolute error was reduced to about 19 %. This accuracy level is similar to that provided by the KETOX hydrodynamic / dispersion model.

2.3 The sediment impact model

2.3.1 General model description

The sediment impact model consists of a series of analytical equations, which may be solved to provide a direct relationship between total contaminant concentration in the water column, and the resulting sediment adsorbed contaminant concentration in the bed layer. As mentioned earlier, the equations are essentially those used by the KETOX toxics sub-model, except for changes made to the partitioning coefficient.

A detailed outline of the theory can be obtained from past reports [3,6]. As a result, only a brief description of the model is provided.

The model simulates the fate and transport of total contaminant, within the water column and bed, as caused by the following transport and transformation processes:

i) settling of suspended solids from the water column to the bed layer,

ii) resuspension of sediment from the bed layer to the water column,

iii) sedimentation of sediment from the bed layer, to a deeper sedimentation layer,

iv) diffusive exchange of water between the water column and bed layer (pore water),

Table 2.4 **Calibration comparison for the " MSOURCE " model.**

Station No.	Measured concentration (ug/L)		Predicted concentration (ug/L), for:						Calibration Error % [1], for River background concentration of 0.3 ug/L, and:		
			No river background concentration, and:			River background concentration of 0.3 ug/L, and:					
	Mean [2]	+/- range [3]	Case 1	Case 2	Case 3	Case 1	Case 2	Case 3	Case 1	Case 2	Case 3
54 A	6.67	0.2	4.9	3.1	3.1	5.2	3.4	3.4	−22	−49	−40
54 B	4	0.2	0	0	0	0.3	0.3	0.3	−92.5	−92.5	−92.5
55	4.21	0.21	4.2	1.3	1.6	4.5	1.6	1.9	6.9	−62	−54.9
56 A	4.6	0.2	3.8	2.9	2.7	4.1	3.2	3	−10.9	−30.4	−34.8
56 B	3.27	0.2	0	0.02	0.15	0.3	0.3	0.5	−90.8	−90.8	−84.7
57	3.07	0.2	2.8	1.33	1.96	3.1	1.6	2.3	1	−47.8	−25.1
58	2.73	0.2	2	1.9	1.6	2.3	2.2	1.9	−15.8	−19.4	−30.4
59	2.47	0.2	1.7	1.6	1.3	2	1.9	1.6	−19	−23.1	−35.2
60	1.86	0.22	1.6	1.5	1.2	1.9	1.8	1.5	2.2	−3.2	−19.4
61 A	1.8	0.2	1.6	1.6	1.4	1.9	1.9	1.7	5.6	5.6	−5.6
61 B	0.8	0.33		< 0.06	< 0.08	0.3	< 0.4	< 0.4	< −50.0	< −50.0	< −50.0
								Average: i) all stations:	−25.9	−42.1	−43
								ii) excluding Stn 54:	−18.9	−35.7	−37.8

LEGEND: Case No. Dispersion factor used: Lateral location of station:

Case No.	Dispersion factor used:	Lateral location of station:
1	0.96	At predicted centre of plume.
2	0.96	As approximated from the field, station map.
3	2	As approximated from the field, station map.

NOTES: [1] Calibration Error =

$$\frac{\{\text{Predicted Concentration} - \text{Measured Concentration}\}}{\{\text{Measured Concentration}\}} * 100\,\%$$

[2] Mean obtained assuming that "non−detected samples" equal to: {detection limit / 2 = 0.5 ug/L }

[3] Range of calculated mean obtained by using extreme values for "non−dectected samples" : { ie. 1 or 0 ug/L }

v) transformation loss (breakdown) of contaminant within the bed layer, (assumed first-order in nature).

It does not account for "horizontal" sediment transport along the surface of the bed layer. This is a useful assumption, since sediment transport is difficult to predict. Further, it does not appear to be a significant factor in reducing large particulate contaminant concentrations within the bed, as caused by ongoing discharges just downstream of point sources, even in areas with strong river currents. For these reasons, it was not considered in the derivation of point source loading limits.

The mathematical description of the sediment impact model are provided via Equations 2.1 through 2.5, as outlined in Appendix I.

The equations as provided, are for a single size class of sediment. However these equations can be easily expanded to incorporate two or more sediment size classes. This is done by including partition coefficients and sediment concentrations for each sediment class. Thus, the total contaminant fraction in particulate form, becomes a summation of the contaminant fractions in each of the individual sediment classes. The equations, as listed in Appendix I, are then modified accordingly. An example of these modifications, for three sediment classes, is provided elsewhere [3].

2.3.2 Input Data

The input data requirements specific to the steady state, bed sediment impact model include: the bed layer porosity and thickness; the settling and resuspension velocities of all sediment types, between the water-column and bed layers; the sedimentation velocity of all sediment types, between the bed layer and deeper sediment layers (in net deposition areas); the partition coefficients for the chemical among all sediment types in both the water-column and bed layers; the mass concentration of each sediment type in both the water-column and bed layers; the diffusion coefficient for dissolved chemical between the water-column and bed layers; and the transformation loss rates of the chemical within the bed layer.

Many of the input data for the model, as listed above, are dependent upon the nature of partitioning of the contaminants of interest. The key requirements include knowledge regarding what type(s) of sediment that the contaminants will adsorb onto, and some measurements of this adsorption. To help address these initial questions, data collected during 1988 by Environments Ontario and Canada were used [14].

In part of this study, Environment Ontario centrifuged river water at 5 "river" stations, (see Figure 2.5). At three of these stations, "whole-water" samples were taken the same day by Environment Canada. Table 2.3 provides a summary of: estimated "particulate" concentrations (assuming a suspended solids concentration of 2 ppm), the average measured "whole-water" concentrations, and the corresponding "particulate" to "whole-water" ratios. In general, this ratio ranges between about .01 to .08 for Zn and Hg, (i.e. about 1 to 8 % of these metals exist

in particulate form within the water-column of the river in the Cornwall vicinity). The ratios for Benzo(a)pyrene are all larger than 1. Since this ratio cannot in reality exceed a value of 1, this may indicate that the "whole water" measured concentrations are too small, perhaps due to a lower extraction efficiency in the sample analysis of this highly hydrophobic parameter. It is quite likely that the actual ratio for Benzo(a)pyrene is well over 0.5 (approaching a value of 1). Only one calculation for PCBs was possible, indicating a ratio of about 0.26.

The water column partitioning coefficient can be estimated by dividing the particulate contaminant concentration measured within the centrifuged sediment, by the total whole water contaminant concentration. The fractions of particulate contaminants within the point source effluents tends to be much higher than those measured at the "river" stations, (refer to Table 2.3). However, these fractions would tend to approach those measured at the "river" stations, due to dilution of the effluent by background river water and suspended sediment. For this reason, only the "river" stations were used to estimate the water column partition coefficients. Overall partition coefficients were estimated by taking the geometric average value from the individual station values. The partition coefficients obtained for: Hg, Zn, and PCBs were: 23900, 17700 and 176000 L_{water} per $kg_{sediment}$; respectively.

The suspended solids concentration in the water column, was set to its estimated average value of 0.9 mg/L (see Table 2.2).

During two MOE field studies in the Cornwall-Massena portion of the St. Lawrence River during 1979 and 1985, the particle size distribution of the bed sediment were measured at several stations, [10,12]. During 1979, the mass fraction distribution (i.e. from gravel to clay) was broken into a total of 8 size classes, whereas 3 were used for the 1985 data.

The total sample mass was not measured during these two field studies. Therefore, the following equation was derived to permit an estimate of the total bed sediment mass concentration, m_2, (i.e. the whole density of in-place bed sediment). It assumes there are 3 sediment size classes, (the 1985 study total):

$$m_2 = \frac{M_2}{V_T} \qquad \ldots\ 2.6a$$

with:

$$M_2 = \frac{D_1 * D_2 * D_3 * (1-POR) * V_T}{(D_2 * D_3 - D_1 * D_3 - D_1 * D_2) * MF_1 + D_1 * D_2 * (1-MF_2) + D_1 * D_3 * (1-MF_3)} \qquad \ldots\ 2.6b$$

where:	D_1, D_2 = D_3	*the densities of the three sediment types, [e.g. in kg/m$_3$]*

$$D_1 = SG_1 * DW$$
$$D_2 = SG_2 * DW$$
$$D_3 = SG_3 * DW$$

SG_1, SG_2, SG_3 = *the specific gravities of the three sediment types*

DW = *the density of water, [e.g. in kg/m$_3$]*

	V_T =	*the total volume of the sample, [e.g. in m$_3$]*
	MF_1, MF_2 = MF_3	*the mass fractions of the sample, as made up by the three sediment types.*

The data from the stations within the north portion of the river (i.e. north of Cornwall and St. Regis Islands), from both 1979 and 1985, were used to estimate the bed sediment concentration. The designations of "1", "2", and "3", were assigned to "sand", "silt", and "clay". The corresponding size classes were: > 62 um, 62 to 3.7 um, and < 3.7 um; respectively. The resulting value obtained (for "bulk" sediment) is 1.37 kg/L. This was calculated based upon the following literature values [3,16,17]:

POR = 0.4
SG_1, SG_2, SG_3 = 2.65, 2.40, 2.00

The concentration of "fine sediments" in the bed, assumed made up of silt and clay only, is 0.549 kg/L.

Settling velocities of the "bulk" and "fine" sediments were assumed equal to about 5.9 and .098 mm/sec [3,16]. Since the point sources discharge into a riverine environment, it is assumed that long-term sedimentation is very small, (i.e. there is very little deposition, since river bathymetry is in an approximate equilibrium state). As a result, a small sedimentation velocity of 1 cm / 100 years was selected.

The resuspension velocity was calculated, using the following equation derived from a sediment mass balance, for the bed layer:

$$w_{rs} = \frac{w_a * m_1 - w_s * m_2}{m_2} \qquad \ldots\ 2.7$$

Using this equation, along with the sediment concentrations and velocities provided above,

estimated resuspension velocities for "bulk" and "fine" sediments are: 3.9×10^{-9} and 1.6×10^{-10}, m/s; respectively.

The diffusion exchange coefficient between the water column and bed layer is not commonly measured. However, it was set equal to 6.1×10^{-6} m/s, based upon similar applications in the past [3,16].

The depth of the bed layer was assumed equal to 3 cm. This is the depth of the surficial bed sediment "Shipek" samples taken during both the 1979 and 1985 MOE field studies [10,12]. These bed sediment data were used in the calibration of the partition coefficients for the bed layer.

2.3.3 Model Calibration

All coefficients used by Eq. 2.5 have been calculated or assigned (as discussed in the previous section), except for the partitioning coefficient within the bed layer, "PC_2". No measurements were made of the contaminant concentration within the pore water of the bed layer, and therefore no direct calculations of the bed layer partitioning coefficient are possible, (i.e. via Eq. 2.2 in Appendix I).

It is reasonable to assume that the partitioning coefficient in the bed layer will be related to that in the water column. Therefore, an appropriate relationship was selected based upon the following general process:

i) Define appropriate equations, which relate "PC_2" to "PC_1" and other sediment properties, and which also incorporate calibration factors.

ii) For each of these equations, select a value of the calibration factor, and obtain "PC_2" for each measurement station.

iii) For each equation and at each measurement station, using "PC_2" and Eqs. 2.4 and 2.2b (of Appendix I); obtain a calculated value for the particulate contaminant concentration in the bed sediment, "r_{2p}", and compare it with the measured value, "r_{2m}". This step requires that the total contaminant concentration in the water column, "C_{T1}", be calculated via use of a hydrodynamic / dispersion model, to account for the relative location of the sediment station with respect to the local upstream point sources.

iv) Obtain the best value of the calibration factor for each partitioning equation, such that the geometric average of all "r_{2p}/r_{2m}" values, (from all available measurement stations), equals 1.

v) Use the "Paired t-test", to determine which calibrated partitioning equation provides the best fit of predicted to measured "r_2".

vi) Readjust slightly the calibration factor, approximate point source loadings and general river background, to improve the quality of the calibration for the selected partitioning equation. ("Slightly" means only as necessary, within the limits of the measured uncertainty).

A total of 4 generic partitioning equations were examined. These are namely:

$$PC_2 = PC_1^A \qquad \text{... 2.8a}$$

$$PC_2 = PC_1 * FF^B \qquad \text{... 2.8b}$$

$$PC_2 = PC_1 * TOC^C \qquad \text{... 2.8c}$$

$$PC_2 = PC_1 * (FF * TOC)^D \qquad \text{... 2.8d}$$

where: *FF* = *the fraction of "fine" sediment in the bulk bed sediment at the station,*

  TOC = *the fraction of total organic carbon in the bulk bed sediment at the station.*

Equation 2.8a attempts to relate "PC_2" directly to "PC_1". Equations 2.8b through d, assume that "PC_2" is related to the fraction of fine sediments and/or total organic carbon, within the bulk bed sediment. The form of these equations are derived in part, upon analysis of bed sediment data as reported in past studies in the Cornwall vicinity [10, 12].

The calibrated KETOX hydrodynamic and dispersion model, was used to predict the total water column contaminant concentrations, at each of the field measurement stations, for each contaminant. This was done using the general river background concentrations, and point source loading rates, as provided in Table 2.2.

The calibration process was programmed using LOTUS 1-2-3 work files. (A separate file was created for each partitioning equation, and for each contaminant). Each of these files summarize and calculate the information for calibration steps "iii) and iv)" above.

The process was carried-out for Hg, Zn, and PCBs. There was not enough measured data to

perform calculations for Benzo(a)pyrene. The "bulk" sediment "m_2" and "w_{rs}" values were used for Eq. 2.8a, whereas the "fine" sediment values were used for Eqs. 2.8b, c, and d. Also, there were no "TOC" measurements made during the 1985 study. As a result, Equations 2.8c and 2.8d could only be applied to the 1979 data.

The calibrated values of the "A", "B", "C" and "D", coefficients (of Eqs. 2.8) obtained for Hg are: .534, 1.99, .63 and .48, respectively. The same calibrated values for Zn are: 1.5, .705, .225 and .171, respectively. Likewise, the same calibrated values for PCBs are: .371, 3.03, 1.07 and .801, respectively.

The "Paired t-test" was used to compare the predicted "r_2" values with the measured "r_2" values, for all 4 equations. Only the 1979 data could be used for the comparison, since Equations 2.8c and d could not be applied to the 1985 data. The tests revealed that the best calibrated equation for all three contaminants, was Eq. 2.8b. This was especially true for Hg and PCBs, but only marginally so for Zn. Using Eq. 2.8b, the calculated "t" values for Hg, Zn, and PCBs are: -0.16, -1.24 and -0.45, respectively, using the combined 1979 and 1985 field data. No significant difference exists between predicted and measured data pairs, at the 5% level of significance.

The final step in the calibration was to "fine tune" the values used for "B" in Eq. 2.8b. This was done after adjusting the river background concentrations and point source loadings for the two sets of data (1979 and 1985), as appropriate to better reflect measured data. This resulted in a better fit for the two data sets individually, as well as combined.

In order to better fit the measured data, it was generally found that the loading from the Domtar diffuser had to be increased for Hg and Zn, and lowered for PCBs, for the 1979 data; with respect to the maximum loading assumed for the calibration as recorded in Table 2.2. Also, the loading from the Courtaulds Storm Sewer, (reflecting near shore discharges from Courtaulds), had to be increased, for all 3 contaminants. The changes required to the river background concentration, with respect to those provided in Table 2, were generally not large, all within a factor of 2.

The LOTUS files for the final calibrated models for Hg, Zn, and PCBs, are provided in Appendix IV. These files summarize the values for: all input parameters, loadings and river background concentrations, comparisons of measured and predicted "r_2" values, and several other parameters of interest.

The final calibrated equations used to define the partitioning coefficient in the bed layer are:

For Hg: $$PC_2 = PC_1 * FF^{2.55} \qquad \ldots\ 2.9a$$

For Zn: $PC_2 = PC_1 * FF^{0.766}$ ... *2.9b*

For PCBs: $PC_2 = PC_1 * FF^{2.52}$ ... *2.9c*

The average, absolute error of predicted bed sediment concentrations (with respect to those measured), is about 108, 88 and 99 %, for the calibrated Hg, Zn and PCBs model, respectively. This is based upon comparison using a total of 39 stations (1979 and 1985 combined) for Hg and Zn, and 34 stations for PCBs. The standard deviation of the ratio of "r_{2p}/r_{2m}" for all stations, is 7.1, 0.9 and 3.0, for the same models, respectively.

2.3.4 Sensitivity Analysis

A sensitivity analysis was conducted in order to gain a qualitative understanding of the behaviour of the model to variations in the values of the input parameters, with respect to the average values used in the calibration. This was done for each contaminant, using the calibrated LOTUS files already developed. The model sensitivity was examined by observing the changes in the geometric average of the "r_{2p}/r_{2m}" ratios, for all available 1979 and 1985 stations, as caused by a change to a given input parameter. Since the measured "r_2" values are constant, any differences in the "r_{2p}/r_{2m}" ratios, are caused by changes in "r_{2p}". The results are summarized in Table 2.5.

There are a total of 12 input parameters for the bed sediment impact model. The sensitivity effect from some of these parameters will be related, since they are used in calculating a common dependent parameter used by the model. For example, "ff", "B" and "PC_1", are all used in obtaining the value for "PC_2". Individually, the 12 input parameters were all decreased and increased in value by a relatively large (but realistic) factor, which varied in value for each parameter.

A "sensitive parameter" may be defined as one that causes a change in the value of the predicted concentration, of approximately the same magnitude as its own change in value (i.e. the model change is proportional, either directly or inversely, to the change in parameter value). Using this general definition, the following "sensitivity classes" may be defined:

Category Name:	*Concentration change / parameter change*
"not sensitive"	*0 to 25 %*
"somewhat sensitive"	*25 to 75 %*
"sensitive"	*75 to 125 %*
highly sensitive"	*over 125 %*

Table 2.5 **Sensitivity analysis results for the sediment model.**

Parameter:		Parameter's Value: (ratio of calibrated)	Geometric average of ratios : r2(predicted) / r2(measured) ; for :		
Name	Symbol		Mercury	Zinc	PCBs
Settling velocity	wa	3.16	1.27	0.98	1.48
		1	1	1	1
		0.316	0.90	1.02	0.71
Pore–water diffusion coef.	k1	10	0.86	1.03	0.58
		1	1	1	1
		0.10	1.84	0.98	2.10
Bed layer thickness	h2	3.16	1.00	1.00	1.00
		1	1	1	1
		0.316	1.00	1.00	1.00
Porosity	h2	2.0	0.53	0.56	0.63
		1	1	1	1
		0.5	1.81	1.66	1.48
Sedimentation velocity	ws	10	1.00	1.00	1.00
		1	1	1	1
		0.10	1.00	1.00	1.00
Total loss–rate in bed layer	k2	half–life 1 mn	0.23	0.089	0.081
		half–life 1 yr	0.71	0.53	0.44
		half–life 10 yr	0.96	0.91	0.87
Conc. of sediment in water–column	m1	3.16	1.22	0.95	1.14
		1	1	1	1
		0.316	0.91	1.03	0.78
Conc. of sediment in bed layer	m2	3.16	1.00	1.00	1.00
		1	1	1	1
		0.316	1.00	1.00	1.00
Fraction of fines in bed layer	FF	2.0	4.01	1.49	2.34
		1	1	1	1
		0.5	0.19	0.64	0.27
Partition coefficient in water–column	PC1	3.16	3.81	3.01	3.61
		1	1	1	1
		0.316	0.29	0.33	0.25
Calibration coef'nt for PC2	B	1.1	0.75	0.92	0.78
		1	1	1	1
		0.909	1.30	1.07	1.24
Total concentration water–column	CT1	3.16	3.16	3.16	3.16
		1	1	1	1
		0.316	0.316	0.316	0.316

It can be seen that the models for Hg and PCBs are "highly sensitive" to changes in "ff", "PC_1" and "B", the 3 parameters used to calculate the bed partition coefficient. The Zn model is "sensitive" to the same 3 parameters. All three models are "sensitive" to "POR". All three models are also "sensitive" and directly proportional to "CT_1", as would be expected by the general form of Equation 2.4. The models are not sensitive at all to "h_2", "w_s", and "m_2". The bed layer depth and sediment concentration would only effect the dynamic aspects of contaminant impact, not the steady-state condition. The sedimentation velocity is too small to effect the results. The model is "somewhat sensitive" to the other three parameters: "w_a", "k_1" and "m_1". It should be noted that "k_2" was assumed equal to 0 for calibration of all three models; therefore the values in Table 2.5 are provided for interest sake only, and are for changes in "k_2" to values representing 3 different half-lives of 1 month, 1 year and 10 years.

Of the three "highly sensitive" parameters, two of them are based upon field measurements (i.e. "ff" and "PC_1"), and the other (i.e. "B") was calibrated. For these reasons, overall model sensitivity should not cause significant problems when using the three models to derive loading limits. This is discussed further in Section 5.

2.4 The Thomann Food Chain model

2.4.1 General model description

The "Thomann food chain model" is the name given to describe a model developed by Dr. R.V. Thomann, of Manhattan College. This model was presented by Dr. Thomann at the Ministry of the Environment's "Aquatic Food Chain Modelling" workshop, in July, 1987 [17].

Details regarding the theory and development of this model are well described within past documents, [17,18]. As a result, only a brief description of the basic features of the model (as provided within these documents) are presented in this report.

The Thomann food chain model was developed to simulate the uptake of hydrophobic, organic chemicals, such as PCBs, which are of concern in the Cornwall area. However, certain locations within this area also experience high levels of Hg in the upper biota trophic levels, and high levels of Zn within the benthos. As a result, and owing to a lack of specific biota impact models and associated biological parameters for heavy metals, the Thomann food chain model was also applied to Hg and Zn. It is reasonable to assume that the model will at least provide approximate results, since the lipid-based partitioning coefficient used in the model is effectively a calibration factor which is used to relate chemical concentration of the organism to that of the water. Therefore, a partitioning coefficient parameter, "PC_1", is used in place of "K_{ow}", for the purposes of this work.

The model is used to estimate the concentration of a chemical within a "one-dimensional", generic aquatic food chain with 4 trophic levels. Biota selected as typical of trophic levels 1 through 4, are: phytoplankton, zooplankton, small fish and large (predator) fish. A schematic diagram showing this "food chain" structure is presented as Figure 2.9. The model calculates

the total bioaccumulation (i.e. due to both water exposure and food consumption), on a lipid basis, for the upper three trophic levels. Chemical concentrations in Level 1 (phytoplankton) are obtained directly from the lipid-based bioconcentration factor, (i.e. partitioning from water).

Chemical uptake into the aquatic food chain is simulated by mathematically representing the pertinent uptake and depuration processes for each trophic level, for "average" specimens, (i.e. a mass balance is used among four average trophic biota, and not on all trophic specimens in the physical system). The basic processes incorporated into the model include: uptake of chemical through respiration; uptake of chemical via food consumption; and reduction of chemical concentration due to chemical excretion and animal growth.

The mathematical description of the Thomann food chain model is provided via Eqs. 2.10 through 2.22, as outlined in Appendix II.

2.4.2 Input data and initial model application

It was first necessary to define which site-specific organisms were to be used in the food chain. Based upon a review of biota sampled by the Ministry of the Environment during 1979 [10] and 1986 [19], and upon a lengthy preliminary modelling exercise which looked at these data, the following decisions were made:

1) Only the 1986 data set would be used, since it was more comprehensive in nature, (i.e. more of the model's input parameters were measured during this study);

2) The (measured) stations to be used for model application were: 366, 368, 368b, 369, 371, 371b, 374, 375 and 398. These stations, the locations of which are provided in Figure 2.10, are those which are impacted by the outfalls under consideration in this study, (i.e. those which lie largely north of Cornwall and St. Regis Islands);

3) Based upon available data, the biota selected to represent Trophic levels 1 through 4 were: attached algae, amphipod, Mottled Sculpin and Brook Trout, (oligochaete was used in-place of amphipod at Station 374, since no amphipod measurements were available there).

This food chain attempted to look at the impacts of in-place (benthic) chemical concentrations upon representative biota in the area. This was also accomplished by selecting amphipods, and more importantly, by using the chemical concentration in the pore water to "drive" the system, as opposed to using the chemical concentration in the water column. This was accomplished by replacing "c_w" used in Equation 2.22 (Appendix II) with "c_s". "c_s" is equivalent to the product of "CT2" and "fd2", (as provided by Eqs. 2.1 and 2.2b in Appendix I).

In order to use the food chain model, eight input parameters must be measured or estimated. Using the symbols already defined in Section 2.4.1 and Appendix II, these parameters are namely: "w", "f_L", "a", "α", "β", "γ", "δ" and "ϕ". The values used for these parameters are summarized in Table 2.6.

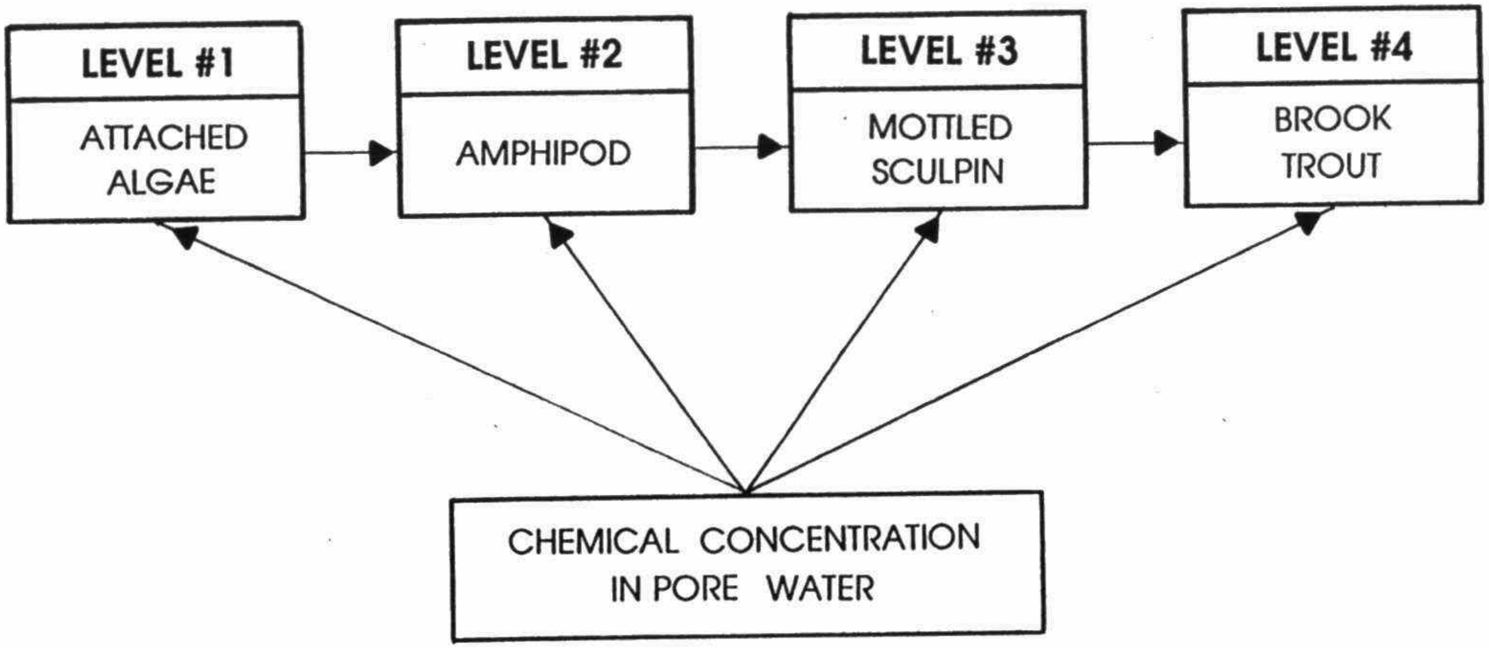


FIGURE 2.9: Food chain structure.

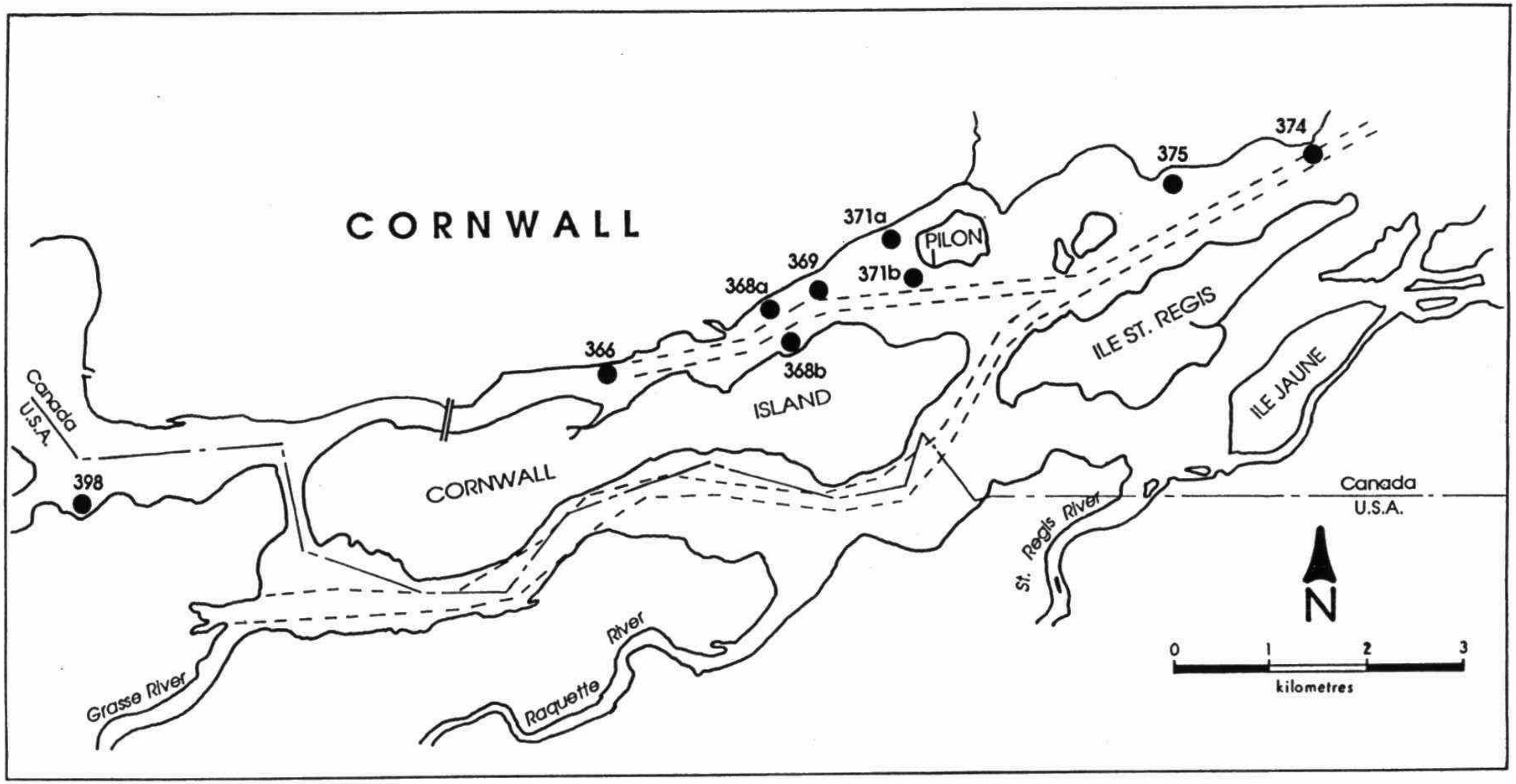


FIGURE 2.10: Biota sampling stations from previous Environment Ontario studies (taken from References 12 and 19)

The weight, "w", of algae, benthic invertebrates and mottled sculpin, were taken or estimated from literature [20,21]. The weight of Small Mouth Bass was based upon measured data [19].

The values used for lipid content, "f_L", were based upon measured values for benthos [19], and estimated from literature [20,21] for the other biota.

The values used for the other 6 parameters, "a", "α", "β", "γ", "δ" and "ϕ", were based upon previous model applications, [18, 22].

2.4.3 Model calibration

The three parameters which logically require some calibration for each chemical, are: the partitioning coefficient, "PC_l"; the chemical assimilation efficiency, "α"; and the efficiency of chemical transfer in the gills, "E". "PC_l" directly affects the basic chemical partitioning to the first trophic level and the "BCF" value for all trophic levels.

The two parameters, "α" and "E", directly affect the ultimate uptake of chemical via the food consumption and respiration routes, respectively. Therefore, possible adjustment of these two factors was considered, (with respect to their "basic values" already discussed in Sections 2.4.2 and Appendix II, respectively). This is accommodated by introducing calibration factors, "EFACTR" and "ALFFTR", to permit alteration of the "basic values".

A "calibration work sheet" was developed via "Lotus 1-2-3", to: record all input data, calculate model parameters, and compare predicted to measured chemical body burdens in the organisms. This was done for all 9 stations where measurements were taken during 1986, (as discussed in Section 2.4.2). The geometric average and standard deviation of all predicted/measured concentration ratios, are calculated and recorded in the work sheet.

To calibrate the model, the calibration factors were adjusted until the geometric average of predicted/measured concentrations equalled one. Where multiple combinations of calibration factors could result in a geometric average of one, the combination providing the lowest standard deviation was assumed to represent the "best fit".

Available measured body burdens of all three chemicals were available for amphipods / oligochaetes, and zinc and mercury body burdens for Mottled Sculpin.

The calibration results are summarized in Table 2.7. The LOTUS files for the final calibrated models are provided in Appendix V. The standard deviation of predicted/measured concentrations are: 74, 115 and 63 %; for mercury, zinc and PCBs, respectively. The total number of predicted-measured data pairs for comparison for these three chemicals were: 18, 18 and 9, respectively.

A "paired t-test" was carried-out on the predicted-measured pairs of data. The calculated "t" values obtained for Hg, Zn and PCBs are: 0.43, 1.02 and 0.70, respectively. Therefore, no

Table 2.6 Parameter values for the food chain model.

Trophic Level	Common name of species	Parameter Name :	wet weight	lipid fraction	food assim. eff.	chemical assim. eff.	empirical coefficients for growth and respiration equations :			
		Symbol	W	LIP	A	ALF *	BETA	GAM	DEL	FI
		Units	gm	–	–	–	–	–	–	–
1	attached algae		0.0002	0.023	0.1	0.1	0.2	0.2	0.01	0.036
2	amphipod / oligochaete		.0023 – .016	.003 – .016	0.3	0.3	0.2	0.2	0.01	0.036
3	Mottled Sculpin		1.8 – 4.1	.033 – .040	0.8	0.8	0.2	0.2	0.01	0.036
4	Brook Trout		128 – 313	.045 – .092	0.8	0.8	0.2	0.2	0.01	0.036

* Note: These are initial values for "ALF", before calibration.

Table 2.7 Calibration results for the food chain model.

Chemical	Calibration parameter value:			Trophic Level	Common name of species	Resulting value of: *	
	PC1 Lw/kglip	EFACTR	ALFFTR			E	ALF
Mercury	15421	1	1	1	attached algae	0.31	0.31
				2	amphipod / oligochaete	0.31	0.31
				3	Mottled Sculpin	0.31	0.31
				4	Brook Trout	0.50	0.50
Zinc	457088	0.032	1	1	attached algae	0.0256	0.0256
				2	amphipod / oligochaete	0.0256	0.0256
				3	Mottled Sculpin	0.0256	0.0256
				4	Brook Trout	0.016	0.016
PCBs	1205036	1	1	1	attached algae	0.7236	0.7236
				2	amphipod / oligochaete	0.7236	0.7236
				3	Mottled Sculpin	0.7236	0.7236
				4	Brook Trout	0.4783	0.4783

* Note: The base value of "ALF" is assumed equal to the "E" value obtained from Eqs. 2.16 (as recommended by Thomann)
Therefore: E = E(from Eq. 2.16) * EFACTR
ALF = E(from Eq. 2.16) * EFACTR * ALFFTR

significant difference is found between predicted and measured data pairs, at the 5% level of significance.

In terms of the geometric average for the two trophic levels, the calibrated mercury model tended to underpredict the benthic body burdens, and over predict those of the Mottled Sculpin, (by approximately 8 %). In order to obtain geometric averages of 1 for the two trophic levels for zinc, a very low "EFACTR" value had to be used, (i.e. only 3.2 % of the "basic values" obtained from Equations 2.16). This is likely due to a relatively large depuration rate for zinc, as compared to the other chemicals, (i.e. the "net" uptake from water is low, since total depuration is large as compared with total uptake).

2.4.4 Sensitivity analysis

A sensitivity analysis was conducted in order to gain a better understanding of the sensitivity of model output, to reasonable changes in the values of the input parameters. The parameters varied include: lipid fraction, lipid-based partitioning coefficient, chemical assimilation efficiency, efficiency of chemical transfer in the gills, growth rate and respiration rate. These parameters were each increased and decreased by factors of 2.

The calibrated models discussed in 2.4.3, were used as the "standard" or base conditions, for comparison purposes. The results are summarized in Table 2.8. Using the sensitivity classification scheme outlined in Section 2.3.4, it can be seen from the table that the food chain model is "sensitive" to "highly sensitive" to changes in the value of lipid fraction and lipid based partitioning coefficient, (since changes in the predicted concentrations are of the same or larger magnitude, to the changes in these parameters), for all three chemicals.

The mercury model is "not sensitive" to changes in the other 4 parameters (growth, respiration and uptake efficiencies), since a change in these parameters' values by +/- 100 % only results in changes to the predicted results of less than 5 %).

The zinc model is "not sensitive" to the growth rate, but is "somewhat sensitive" to changes in the respiration rate, and is "sensitive" to changes in the uptake efficiencies.

The PCBs model is "not sensitive" to changes in the gill uptake efficiency and growth rate, but is "somewhat sensitive" to changes in the food chemical uptake efficiency and respiration rate.

In general, it appears that the sensitivity of the food chain model increases, as the lipid-based partitioning coefficient of a chemical increases. It is also likely that inaccuracies in the measured / estimated lipid fractions, particularly between trophic levels, have contributed to the errors (as indicated via the standard deviations) in the accuracy of the predictions. It is therefore important to have accurate estimates of lipid-based partitioning coefficient and lipid contents for the model.

Table 2.8 Sensitivity analysis results for the food chain model.

Parameter:		Parameter's Value: (ratio of calibrated)	Geometric average of ratios : r2(predicted) / r2(measured) ; for :		
Name	Symbol		Mercury	Zinc	PCBs
Fraction of lipid	fL	2	2.05	2.38	3.20
		1	1	1	1
		0.5	0.50	0.40	0.33
Partitioning coef. in water	PC1	2	2.01	1.91	2.72
		1	1	1	1
		0.5	0.50	0.59	0.40
Assimilation effic'y of chemical in food	alf	2	1.03	1.88	1.72
		1	1	1	1
		0.5	0.99	0.67	0.64
Transfer efficiency of chemical in gills	E	2	1.03	1.79	1.16
		1	1	1	1
		0.5	0.96	0.53	0.83
Net, relative growth rate	G	2	1.01	0.84	1.08
		1	1	1	1
		0.5	1.00	1.24	0.95
Relative respiration rate	r	2	1.02	1.67	1.56
		1	1	1	1
		0.5	0.99	0.74	0.72

2.5 The Thomann Foodweb model

2.5.1 General model description

The "Thomann foodweb model" is the name given to describe a model developed subsequently to the "Thomann food chain model", by Dr. R.V. Thomann of Manhattan College. Dr. Thomann presented some applications of this model at the "6th Colloquium on Pulp and Paper Mill Effluents", in December, 1991 [23]. He also kindly sent a copy of a detailed manuscript of this model which has now been published [24]. This published manuscript should be referred to in order to gain a comprehensive understanding of the derivation of the model. However, the following is presented as a brief description of the primary features.

The foodweb model is generally similar to the food chain model described in Section 2.4.1. However, in addition to the 4 basic trophic levels (called compartments), it also includes a benthic invertebrate compartment. Further, there are several addition chemical exposure routes considered by the foodweb model, as follows:

i) The benthic invertebrates may accumulate chemical from either the water column or bed layer, or both, via: ventilation of water from the water column and/or pore water in the bed sediment; and ingestion of bed sediment organic carbon and/or phytoplankton/detritus material.

ii) The forage fish may accumulate chemical from ingestion of zooplankton and/or benthic invertebrates, (as well as ventilation within the water column).

These chemical exposure routes are shown schematically in Figure 2.11.

The fractions of the total food and water which the benthic invertebrates consume coming from the water column and bed layer, are adjustable in the model. Likewise, the fraction of the total food supply which the forage fish consume coming from zooplankton and benthic invertebrates, is also adjustable.

The basic mass balance equation used to describe the uptake of chemical into zooplankton and piscivorous fish in the foodweb model, (i.e. Compartments Nos. 2 and 4, respectively), is similar to the general equation used in the food chain model, (i.e. Equation 2.10). Similar to the food chain model, the foodweb model assumes simple partitioning to describe the steady-state concentration of chemical within phytoplankton, (i.e. Compartment No. 1). However, to describe the uptake of chemical into benthic invertebrates and forage fish, the foodweb model uses a modified equation to accommodate the multiple exposure routes for these biota.

The mathematical description of the Thomann foodweb model is provided via Eqs. 2.23 through 2.36, as outlined in Appendix III.

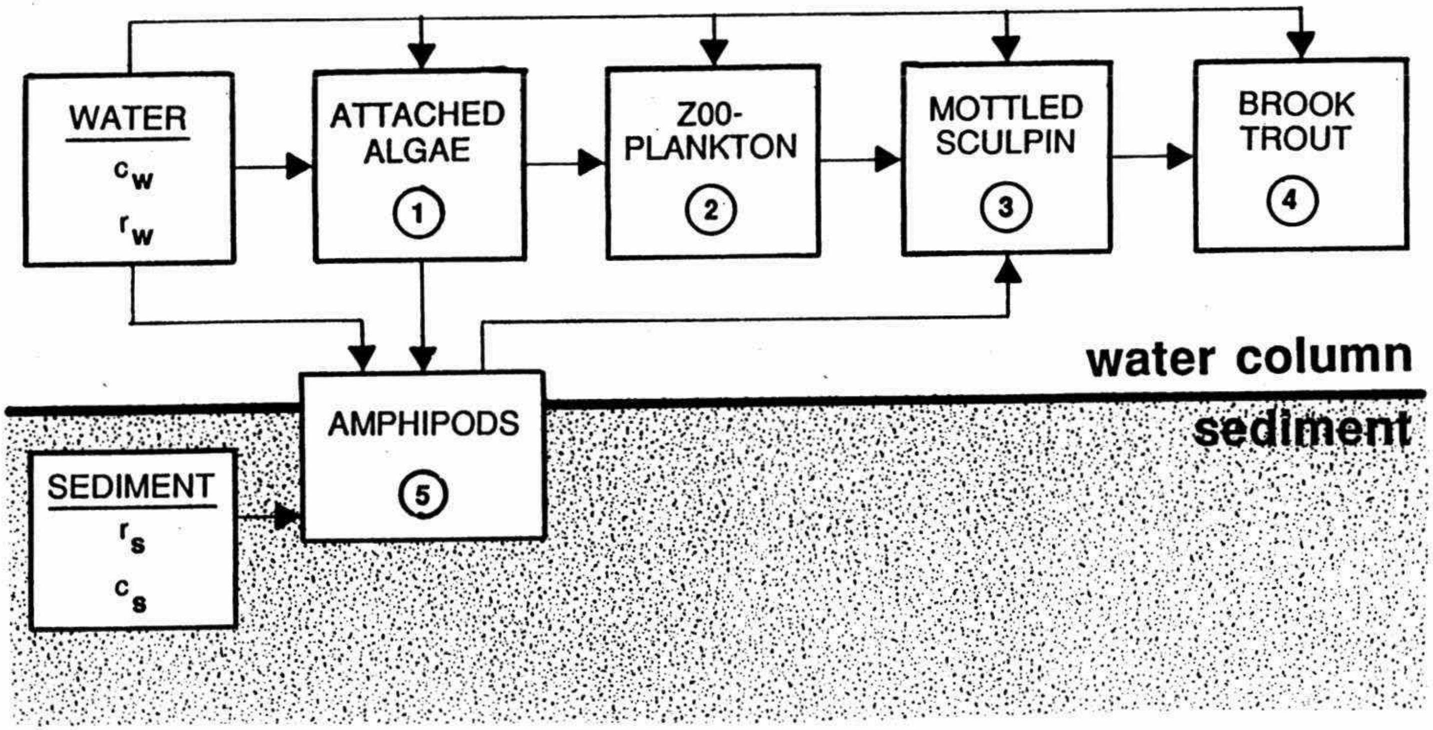


FIGURE 2.11: Food web structure.

2.5.1.1 Accommodation of methylmercury:

It is widely believed that methylmercury is the main speciated form of mercury which is accumulated by biota. Therefore, it is desirable for the foodweb model to be able to look at only a specified fraction of the total mercury. However, it is necessary for the water column and sediment models discussed earlier, to simulate total mercury, since available loading and ambient concentration data usually are reported for this form only. As a result, "bioavailable factors", ("fmm_{cw}", "fmm_{cs}" and "fmm_{rs}"), were introduced into the foodweb model for mercury. They permit the use of only a specified portion of the total mercury exposure concentrations, for estimating uptake into the food web. These factors have the form of:

$$fmm_{ii} = \frac{Cmm_{ii}}{Ctm_{ii}} \qquad \ldots\ 2.37$$

where: *Cmm = concentration of methylmercury,*

Ctm = concentration of total mercury, and

ii = exposure compartment, where:

cw = dissolved form in water column,
cs = dissolved form in bed layer, and
rs = particulate form in bed layer.

The mercury foodweb model does not perform a mass balance upon methylmercury, but simply allows a fraction of the total mercury (which is subject to mass balance) to be assigned as methylmercury, for the three exposure compartments listed above.

2.5.2 Input data and initial model application

The various mathematical algorithms and input/output data requirements of the model were programmed using FORTRAN-77. A source code listing is provided in Appendix VIII. The computer program was tested, using the Lake Ontario data base reported by Dr. Thomann [24], (i.e. to assure no coding errors existed, the computer program was run to reproduce the results of the Lake Ontario application).

The foodweb model was then applied to the same measured MOE-Cornwall data base, (see Section 2.4.2). To do this, the model was reprogrammed onto a "Lotus 1-2-3" data file, to permit a more "user friendly" environment.

The specific biota selected to represent the 5 compartments, in sequential order, are: attached algae, zooplankton, Mottled Sculpin, Brook Trout, and amphipods (oligochaetes at Stn 374).

In addition to the 8 input parameters required for the food chain model, the foodweb model requires an additional 5 parameters to be defined. They include: "A_{wd}", "A_{oc}", "A_c", "O_2" and "K_1", (see Eqs. 2.25 and 2.26).

The values used for all input parameters are summarized in Table 2.9. The values used for "A_{wd}", "A_{oc}", and "A_c", were based upon the Lake Ontario application [24]. The value of "O2" used was 8.5 mg/L. The value of "K_1" was assumed to require calibration.

In addition, the concentration of the chemical in particulate form within the bed layer, ("r_2"), along with the fractions of organic carbon within both bed sediment and suspended sediment, ("f_{ocs}" and "f_{ocw}"), are required. "r_2" and "f_{ocs}" were measured at the stations of interest [10,12]. "r_2" is also predicted by the sediment impact model, (see Eq. 2.4 in Appendix I). "f_{ocw}" was set equal to 5 times "f_{ocs}", based upon past general observations.

Levels of methylmercury within the bed sediment were measured by the MOE during 1991, [25]. The results indicate that approximately 1 % of the total mercury is made up of methylmercury. As a result, "fmm_{rs}" was set equal to 0.01. Also, due to a lack of measurements, but accounting for sediment / water exchange with the water column, "fmm_{cs}" and "fmm_{cw}" were also set as 0.01.

2.5.3 Model calibration

The parameters which were considered subject to calibration include: the lipid-based partitioning coefficient, "PC_1"; the fecal and metabolism loss factor, "K_1"; and the various ventilation volume and mass consumption fractions, for Compartments 5 and 3, (ie. "b_{5s}", "b_{5w}", "p_{5s}", "p_{51}", "p_{32}" and "p_{35}"), since no specific measured data were available to determine these values.

The model was calibrated (for each chemical separately), using a "Lotus 1-2-3" worksheet specially developed for this purpose. As for the food chain model, predicted versus measured chemical body burdens were compared with measured data where available, (as discussed in Section 2.4.3, with the exception of Station 398). The geometric average and standard deviation of all predicted/measured concentration ratios, are calculated and recorded in the work sheet.

Since there were several potential calibration factors as listed above, a "two-stage calibration" was performed, as follows:

1) the calibration coefficients were placed in two groups, according to their general nature. "PC_1" and "K_1" were grouped together, since they deal most directly with chemical uptake and loss. The other group consisted of the volume and mass consumption factors;

2) it was assumed that the food consumption and respiration volume fractions for benthic invertebrates were equal, as follows:

$b_{5s} = p_{5s}$ and $b_{51} = p_{51}$;

3) for a given set of values for the volume and mass consumption factors, the "PC_1" and "K_1" values were adjusted to produce a predicted to measured geometric average of 1, (i.e. both for the overall data set, and for each compartment's data); and

4) the combination of calibration parameters, resulting in the lowest standard deviation of predicted to measured concentration ratios (i.e. the "best fit"), was deemed to represent the "calibrated" condition.

The calibration results are summarized in Table 2.10. The LOTUS files for the final calibrated models are provided in Appendix VI. The standard deviation of predicted/measured concentrations are: 76, 92 and 80 %; for methylmercury, zinc and PCBs, respectively. The total number of predicted-measured data pairs for comparison for these three chemicals were: 16, 16 and 8, respectively. In addition, the geometric average of predicted/measured ratios equals 1 for both measured biota compartments (for methylmercury and zinc where two biota compartments were measured).

A "paired t-test" was carried-out on the predicted-measured pairs of data. The calculated "t" values obtained for Hg, Zn and PCBs are: -0.79, 0.73 and -0.57, respectively. Therefore, no significant difference is found between predicted and measured data pairs, at the 5% level of significance.

The standard deviation of predicted/measured concentrations, using "total mercury" (instead of methylmercury), is about 104 %. In addition, the geometric average of predicted/measured concentrations for Compartments 3 and 5 are about 0.85 and 1.16 respectively, (i.e. the model underpredicted and overpredicted concentrations in Compartments 3 and 5, respectively). Thus, there is an improvement in model accuracy by attempting to simulate methylmercury uptake in biota, as opposed to total mercury.

2.5.4 Sensitivity analysis

A sensitivity analysis was conducted in order to gain a better understanding of the sensitivity of model output, to reasonable changes in the values of the input parameters. The parameters considered in this analysis for all chemicals include: lipid fraction, lipid-based partitioning coefficient, chemical assimilation efficiency, efficiency of chemical transfer in the gills, growth and respiration rates, ventilation volume fraction for the benthos, and food consumption mass fractions for the benthos and forage fish. In addition, the non gill-membrane, chemical loss rate is also considered for methylmercury and zinc. Finally, the bioavailable mass fractions (i.e. the ratio of methylmercury to total mercury) are also considered.

The calibrated models discussed in 2.5.3, were used as the "standard" or base conditions, for comparison purposes. The sensitivities were classified according to the general definition provided in Section 2.3.4. The results are summarized in Table 2.11. The biota concentrations for all chemicals are "highly sensitive" to changes in the value of lipid fraction and lipid based

partitioning coefficient, and "somewhat sensitive" to changes in the breathing volume fractions for benthos.

The methylmercury model is "sensitive" to the bioavailable concentration dissolved in the water column, "somewhat sensitive" to the food mass consumption fractions for benthos, and "not sensitive" to the bioavailable concentrations within the bed layer.

The biota concentrations are "not sensitive" to changes in the value of the chemical transfer efficiencies, growth and respiration rates, the food mass consumption ratios for forage fish, and the non gill-membrane chemical loss rate.

3. WATER, SEDIMENT AND BIOTA CRITERIA AND GUIDELINES

The concentration criteria used in the load allocation procedure are summarized in Table 3.1. These are for concentration levels in three media: water (in water-column), sediment (in bed layer), and aquatic biota tissues (chemical body burden).

3.1 Water criteria

"Provincial Water Quality Objectives", (PWQOs), were used for all contaminants [31]. The criterion used for benzo(a)pyrene, is a "Provincial Water Quality Interim Guideline" (PWQIG).

It was assumed that the maximum permitted increase in suspended solids concentration was 10 % of the general river background value. (A conservative estimate only, assuming that turbidity and suspended solids are linearly correlated.)

3.2 Sediment criteria

The "Provincial Sediment Quality Guidelines" (PSQGs) were used to provide criteria for contaminant levels in the sediment of the bed layer [32,33]. PSQGs were developed to provide for the protection of aquatic biological resources. The guidelines considered included those associated with two levels of ecotoxic effects:

i) A "Lowest Effect Level" (LEL), which is "a level of sediment contamination at which the majority of benthic organisms are unaffected" [32,33], and

ii) A "Severe Effect Level" (SEL), which is "the level at which pronounced disturbance of the sediment-dwelling community can be expected." [32,33].

Criteria were available for only mercury, zinc and PCBs.

The ways in which these two levels of criterion are used, are described in Sections 4 and 5.

Table 2.9 Parameter values for the foodweb model.

Compartment number	Common name of species	Parameter Name :	wet weight	lipid fraction	food assim. eff.	chemical assim. eff.	empirical coefficients for growth and respiration equations :			
		Symbol	W	LIP	A	ALF	BETA	GAM	DEL	FI
		Units	gm	–	–	–	–	–	–	–
1	attached algae		0.0002	0.023	0.1	0.8	0.2	0.2	0.01	0.036
2	zooplankton		0.01	0.05	0.3	0.8	0.2	0.2	0.01	0.036
3	Mottled Sculpin		1.8 – 4.1	.033 –.040	0.8	0.8	0.2	0.2	0.01	0.036
4	Brook Trout		128 – 313	.045 – .092	0.8	0.8	0.2	0.2	0.01	0.036
5	Amphipods / Oligochaetes		.0023 –.016	.003 – .016	0.2	0.8	0.2	0.2	0.01	0.036

Compartment number	Common name of species	Parameter Name :	wet/dry ratio	oxygen to carbon ratio	carbon/dry ratio	[Oxygen] in water
		Symbol	Awd	Aoc	Ac	O2
		Units	–	–		mg/L
1	attached algae		0.0002	0.023	0.1	8.5
2	zooplankton		0.01	0.05	0.3	
3	Mottled Sculpin		1.8 – 4.1	.033 –.040	0.8	
4	Brook Trout		128 – 313	.045 – .092	0.8	
5	Amphipods / Oligochaetes		.0023 –.016	.003 –.016	0.2	

Table 2.10 Calibration results for the foodweb model.

Chemical	Calibration parameter :	Partitioning coefficient	Non–gill loss–rate	Benthic invertebrates' ventilation fraction from:		Benthic invertebrates' food fraction from:		Forage fish's food fraction from:	
				porewater	water–col.	bed layer	water–col.	bed layer	water–col.
	Symbol	PC1	K1	b5s	b5w	p5s	p51	p35	p32
	Units	Lw / kglip	1/day	–	–	–	–	–	–
Mercury		654,636	0.0181	0.1	0.9	0.1	0.9	0.5	0.5
Zinc		91,620	0.149						
PCBs		676,100	0						

Table 2.11 Sensitivity analysis results for the foodweb model.

Parameter: Name	Symbol	Parameter's Value: (ratio of calibrated)	Geometric average of ratios : r2(predicted) / r2(measured) ; for : Methyl-Hg	Zinc	PCBs
Fraction of lipid	fL	2	3.57	2.26	2.88
		1	1	1	1
		0.5	0.29	0.48	0.38
Partitioning coef. in water	PC1	2	3.37	2.25	2.74
		1	1	1	1
		0.5	0.30	0.48	0.38
Assimilation effic'y of chemical in food	alf	2	1.07	1.02	1.00
		1	1	1	1
		0.5	0.90	0.97	1.00
Transfer efficiency of chemical in gills	E	2	1.03	1.04	1.01
		1	1	1	1
		0.5	0.94	0.86	0.94
Net, relative growth rate	G	2	1.12	1.11	1.12
		1	1	1	1
		0.5	0.94	0.95	0.94
Relative respiration rate	r	2	1.07	1.08	0.94
		1	1	1	1
		0.5	0.95	0.91	1.12
Benthic inverteb's ventilation fraction: porewater/wat-col	B5S & B5W	1 & 0	1.21	1.27	1.41
		0.1 & 0.9	1	1	1
		0 & 1	0.98	0.97	0.95
Benthic inverteb's food fraction: bed layer/wat-col	P5S & P51	1 & 0	0.66	2.36	2.77
		0.1 & 0.9	1	1	1
		0 & 1	1.03	0.82	0.71
Forage fish's food fraction: bed layer/wat-col	P35 & P32	1 & 0	1.16	1.07	1.00
		0.5 & 0.5	1	1	1
		0 & 1	0.82	0.93	1.00
Non-gill, chemical loss-rate	K1	2	0.83	0.82	–
		1	1	1	–
		0.5	1.12	1.14	–
Total bed sediment Hg as methyl-Hg	fmmrs	2	1.05	–	–
		1	1	–	–
		0.5	0.98	–	–
Total suspended sediment Hg as methyl-Hg	fmmcs	2	1.04	–	–
		1	1	–	–
		0.5	0.99	–	–
Total dissolved water-column Hg as methyl-Hg	fmmcw	2	1.93	–	–
		1	1	–	–
		0.5	0.54	–	–

Table 3.1 Concentration criteria, and mean river background concentrations.

Parameter	CONCENTRATION CRITERION for:			
	Water [mg/L] [1]	Biota [ug/g] [2]	Sediment [ug/gsed] LEL [3]	Sediment [ug/gsed] SEL [4]
Mercury	0.0002	0.5	0.2	2
Zinc	0.03		120	820
Total PCBs	1.0E−06	0.1	0.07 [5]	18.6 [6]
Benzo(a)pyrene	6.0E−08			
Phenolics	0.001			
Suspended solids	0.99			

Mean, whole−water, river background concentrations, used for the load allocations, [mg/L]:

Mercury	0.00001
Zinc	0.002
PCBs	1.00E−06
BAP	
Phenolics	1.10E−06
Sus. Seds	0.9

Notes:

[1] Water criteria are PWQOs, (Ref. 31), except:
- criterion for B(a)P is a PWQIG ;
- criterion for suspended solids is based on the PWQO for turbidity.

[2] These are the GLWQA guidelines for whole fish (wet weight), to protect fish eating wildlife, (from Ref. 34).

[3] MOEE "Lowest Effect Level", from Ref's 32 and 33.

[4] MOEE "Severe Effect Level", from Ref's 32 and 33.

[5] Based on a limited bed sediment TOC of 1 % .

[6] Based on the actual average bed sediment TOC along the north shore of about 3.5 % (using Ref. 26 data).

3.3 Aquatic biota criteria

The criteria used for aquatic biota are those for fish tissue (whole fish, calculated on a wet weight basis), for the protection of birds and animals which consume fish. These were taken from the "Revised Great Lakes Water Quality Agreement of 1978" [34].

Values were only available for mercury and PCBs.

4. DERIVATION OF CHEMICAL LOADING LIMITS FOR AVERAGE CONDITIONS

Loading limits are derived to comply with each of the 3 types of criterion (water, sediment and aquatic biota) separately, within mixing zones, using the models described in Section 2.

4.1 Regulatory Mixing Zone

The "Regulatory Mixing Zone" (RMZ) may be defined as the physical region downstream of a point source, at the boundaries of which, all chronic concentration criteria for aquatic life protection (whether for water, sediment, or biota) must be achieved. At this point in time, the requirements for defining this zone under various conditions have not been fully established. As a result, the chemical loading limits procedure outlined in this section, will look at various lengths for the "Regulatory Mixing Zone". In consultation with the Cornwall MISA Pilot Site team, the distances considered included 1000, 500, and 200 m downstream from the outfall. In addition, calculations are carried out based upon an RMZ length coinciding with the downstream end of the near field mixing zone, called the ENF for brevity. The ENF is the location where the discharged effluent plume from an outfall, has been vertically mixed sufficiently to cover the entire water column depth. The ENF is generally located about 5 times the river depth, downstream of an outfall in rivers with a strong current [16]. Thus, the ENF should represent distances of from about 15 to 50 m, downstream from the 5 point sources analyzed in this study.

4.2 Loading limits based upon water column impact

4.2.1 Selection of model

As discussed earlier, two hydrodynamic and dispersion models were applied to analyze the impact of discharged contaminants from the Cornwall point sources upon the water column. These two models (KETOX and MULTISOURCE) were evaluated to obtain the best model to use for the load allocation process. To evaluate the models, they were used to predict the percentage of relative concentration within the water column of the river at the end of the "near field mixing zone" (ENF), of the 5 point sources. These results were compared to a calculated percentage of relative concentration obtained using a mass balance procedure. In this mass balance procedure, the effluent discharge is simply divided by the sum of the effluent discharge plus the portion of the river flow impacted by the plume at the ENF.

The results of the comparisons are provided in Table 4.1. Both models predict similar results to each other and to the calculated relative concentration percentage (i.e. within a factor of 2), for the Domtar / CIL / Cornwall Chemical Diffuser. This fact is also reflected in the good calibration results of phenolics (based mainly on discharges from this diffuser), discussed earlier. The MULTISOURCE model accurately predicts the ENF concentrations for the other 4 outfalls as well, (i.e. always within a factor of 2). However, the KETOX model tends to under predict the ENF concentration for the other 4 outfalls (i.e. the mass balance values are from 2.5 to 34 times larger than those predicted by the KETOX model). The reason for the ENF underprediction is explained almost entirely by the size of the grid discretization used by the KETOX model. Table 4.1 shows that: the ratio of relative concentration predicted by the KETOX model divided by the relative concentration calculated by the mass balance method; is almost equivalent to the ratio of the ENF width, divided by the KETOX model's discretization width at the outfall, (i.e. Column "6a" is similar to Column "8").

In conclusion, it can be said that the lateral grid size to be used to provide accurate ENF results, should be no wider than approximately the width of the ENF. In the case of the Courtaulds extended storm sewer ENF, the required grid size is about 2.5 m. Since the MULTISOURCE lateral grid size used was 3.0 m, it was able to accurately predict the ENF concentrations.

From this analysis, it was decided to use the MULTISOURCE model for allocating loads based upon water column criterion, in the region nearest the outfalls (e.g. within 1 kilometre). However, it should be stated that the KETOX model could be used to provide more accurate results, by modelling only a portion of the river channel at a time, and thus using a finer grid size. This was successfully done for the St. Clair MISA Pilot load allocation work [16]. Also, the KETOX model more accurately predicted the general dispersion pattern in the regions farther downstream from the outfalls, especially where the river flow exhibits curvatures and widening (near Pilon Island).

4.2.2 General dispersion results

The MULTISOURCE model was used to predict the concentrations of a conservatively behaving contaminant, at all 4 mixing zone lengths downstream of each of the 5 point sources, for:

- a 1 kg/day steady loading rate, under an approximate average effluent flow-rate;

- the long-term average flow-rate in the river channel north of Cornwall Island, of about 2180 cms.

The results are provided in Table 4.2. As can be derived from this table; the minimum near field dilution obtained at the ENF (at the centre of the plume) of the Domtar diffuser, Courtaulds Viscose and Acid Diffusers, Courtaulds extended storm sewer, and Cornwall WPCP diffuser, is about: 124, 807, 958, 33, and 45, respectively. These values provide an indication of the relative dispersive characteristics of the river in the immediate vicinity of the point source discharge locations.

Table 4.1 Comparison of results from the " KETOX " and " MSOURCE " models.

Point Source	Total Effluent:		Approximate River:		Relative Concentration (%) at the ENF, by:			Ratio of:		Nodal Spacing (m)		Ratio of:
	Discharge Width (m)	Flow Rate (m^3/sec)	Depth (m)	Velocity (m/sec)	Mass Balance	KETOX	MSOURCE	Col. {5b} ----- Col. {5a}	Col. {5c} ----- Col. {5a}	KETOX	MSOURCE	Col. {1} ----- Col. {7a}
{Column #}>	{1}	{2}	{3}	{4}	{5a}	{5b}	{5c}	{6a}	{6b}	{7a}	{7b}	{8}
Domtar/CIL/ Cornwall Chem. Diffuser	48	1.53	2.6	2.8	0.436	0.483	0.8	1.11	1.83	38	3.05	1.26
Courtaulds – Viscose/Sulphide Diffuser	12	0.107	8.5	0.7	0.15	0.062	0.124	0.41	0.83	32	3.05	0.38
Courtaulds – Acid Diffuser	12	0.082	8.5	0.7	0.115	0.047	0.104	0.41	0.9	32	3.05	0.38
Courtaulds – Storm Outfall	2.5	0.063	4.6	0.3	1.793	0.052	2.941	0.029	1.64	76	3.05	0.033
Cornwall WPCP Diffuser	15	0.564	7.3	0.4	1.271	0.324	2.169	0.25	1.71	68	3.05	0.22

Table 4.2 Concentrations within the river, at different downstream distances along the plume centreline, caused by a 1 kg/day loading rate from the source outfall.

Source Outfall	EFFLUENT		CONCENTRATION (ug/L), above background, due to a 1 kg/day load, at downstream distances (m), of :			
	Flow [cms]	Conc. [ug/L]	ENF	200	500	1,000
Domtar/CIL/Cornwall Chemical Diffuser	1.53	7.56	0.061	0.0445	0.0413	0.0348
Courtaulds – Viscose/Sulphide Diffuser	0.107	108.2	0.1341	0.0464	0.0388	0.0303
Courtaulds – Acid Diffuser	0.082	141.1	0.1473	0.0415	0.0328	0.0269
Courtaulds – Storm Outfall	0.063	183.7	5.5	0.957	0.747	0.522
Cornwall WPCP Diffuser	0.564	20.5	0.4545	0.1667	0.1035	0.0563

The minimum "far field" dilution, occurring along the centre of the plume between the ENF and a distance of 1 km, is also indirectly provided in Table 4.2. This additional dilution, (i.e. over and beyond that provided between the diffuser or outfall and the ENF); for the Domtar diffuser, Courtaulds viscose and acid diffusers, Courtaulds extended storm sewer, and Cornwall WPCP diffuser, is about: 1.8, 4.4, 5.5, 11 and 8.1, respectively.

4.2.3 Generalized background concentrations from upstream point sources

As part of the load allocation process, it is necessary to determine the maximum loading rates so as not to exceed various concentration criteria at downstream locations. However, the concentration at a given location downstream from a point source is a sum of the concentrations due to both the point source itself, and any existing background concentration. This background concentration is a sum of two portions. These are namely the general river background concentration (i.e. due to very distant point and non-point sources), and the other local, upstream point sources. It is thus necessary to ascertain from simulation models, the concentrations of discharged point source contaminants at the downstream locations of other point sources involved in the load allocation procedure.

The distances between the Domtar and Cornwall WPCP diffusers, is about 5.5 km. Also, the Cornwall river channel exhibits significant bending and widening between these point sources. In addition, the Cornwall WPCP diffuser is situated close to the "edge" of the effluent plume from Domtar. Under these conditions, as discussed in the calibration portion of the report, the KETOX model was found to perform better. Thus the KETOX model was used to provide concentrations at the Cornwall WPCP diffuser from upstream sources, with the MULTISOURCE model used to provide the other impacts, (where both models showed similar results).

The impact results, as listed in Table 4.3, are based upon a steady discharge rate of 1 kg/day, of a conservatively behaving contaminant, from the "source" (upstream) point source.

4.2.4 Maximum Allowable Loads

The maximum allowable load for a particular chemical, from a given outfall, is defined as the load which creates a total chemical concentration which is equivalent to the concentration criterion, at the end of the "regulatory mixing zone" (RMZ).

The total contaminant concentration that will exist at the end of the RMZ, downstream from a particular outfall, is the summation of the contributions due to: the particular outfall itself, plus the individual "local" upstream sources whose plumes also impact the same point, plus the general river background. Written in equation form, this relationship is as follows:

$$C_{tn} = A_n * L_n + \sum_{i=1}^{n-1} (A_{i,n} * L_i) + C_{rb} \qquad \ldots\ 4.1$$

where:

n = *the assigned integer number, of the particular outfall being analyzed.*

i = *the assigned integer number given to identify each outfall within a group of "N" "local" outfalls. These "local" outfalls are numbered sequentially, (i.e. 1,2,3,...,N), moving in the downstream direction.*

C_{tn} = *the total contaminant concentration, at the end of the RMZ of outfall "n", [e.g. in ug/L].*

L_n = *the contaminant loading rate, discharged from outfall "n", [e.g. in kg/day]*

L_i = *the contaminant loading rate, discharged from a given "local" upstream point source "i", [e.g. in kg/day]*

A_n = *the contaminant concentration at the end of the RMZ of outfall "n", due to a unit loading rate from outfall "n", [e.g. in (ug/L)/(kg/day)]*

$A_{i,n}$ = *the contaminant concentration at the end of the RMZ of outfall "n", due to a unit loading rate from a given "local" upstream source "i", [e.g. in (ug/L)/(kg/day)]*

C_{rb} = *the general river background concentration of the chemical, due to distant upstream, well dispersed sources, [e.g. in ug/L].*

Functionally, there are two basic characteristics that would distinguish the "general river background concentration", from those due to "local" upstream point sources. These include:

i) The general river background concentration is well mixed laterally within the portion of the river where the outfall in question is being analyzed.

ii) The general river background concentration is not directly identifiable or controllable, for purposes of the loading limits exercise.

Incorporating contaminant background concentrations into the loading limit process, may or may

Table 4.3 Concentration within the river at each downstream outfall, caused by a 1 kg/day loading rate from the source outfall.

Source Outfall	Source's Effluent: Flow	Source's Effluent: Conc.	CONCENTRATION (ug/L); caused by a 1 kg/day load from the source outfall; AT OUTFALL:			
	[cms]	[ug/L]	II.	III.	IV.	V.
I. Domtar/CIL/Cornwall Chemical Diffuser	1.53	7.56	0.0069	0.0069	0.0129	0.0058
II. Courtaulds – Viscose/Sulphide Diffuser	0.107	108.2			0	0.0101
III. Courtaulds – Acid Diffuser	0.082	141.1			0	0.0101
IV. Courtaulds – Storm Outfall	0.063	183.7				0.0038
V. Cornwall WPCP Diffuser	0.564	20.5				

not be necessary, depending upon their relative magnitude, at the end of the RMZ. In order to examine their potential impact upon the resulting maximum loading limits, three cases are considered. These include:

Case I: Neither the general river background chemical concentration, nor those due to local upstream point sources, are considered.

Case II: Only the general river background chemical concentration is considered.

Case III: Both the general river background chemical concentration and the concentrations due to all local upstream point sources, are considered.

Mathematically, the maximum allowable load derived for these three cases are represented as:

Case I: $$L_{1maxn} = \frac{C_{crit}}{A_n} \qquad \ldots 4.2$$

Case II: $$L_{2maxn} = \frac{C_{crit} - C_{rb}}{A_n} \qquad \ldots 4.3$$

Case III: $$L_{3maxn} = \frac{C_{crit} - C_{rb} - \sum_{i=1}^{n-1} (A_{i,n} * L_i)}{A_n} \qquad \ldots 4.4$$

where: L_{1maxn}, L_{2maxn}, L_{3maxn} = *the maximum allowable load of chemical from outfall "n", (e.g. in kg/day), for Cases I, II, & III, respectively.*

C_{crit} = *the chemical's concentration criterion, to protect the receiving water body, (e.g. in ug/L)*

4.2.4.1 Case I: No background concentrations:

The derived maximum allowable loads in this case are summarized in Table 4.4. These were obtained using Equation 4.2. Under this assumption, the water column criteria used to calculate the maximum allowable loading rates, does not need to be reduced (to reflect an existing concentration within the water column upstream of the given point source).

There are some general characteristics illustrated by the allocated loads as listed within Table 4.4. These include:

i) The ratio of the different allocated loads, for the different contaminants, at the same outfall and mixing zone distance; are simply equal to the ratio of their respective water quality criterion used in the analysis.

ii) The ratio of different allocated loads, for the same contaminant and mixing zone length, but at the different outfalls; are equal to their respective ratios of plume dilutions.

iii) The different ratios of allocated loads for different mixing zone lengths of the same outfall, with respect to those from another outfall; are caused by differences in the far field to near field dilution ratios. This in turn is a function of the initial outfall configuration. For example the ratio of allocated loads at 1000 m to that at the ENF, is less than 2 for the Domtar diffuser, whereas it is over 10 for the Courtaulds Storm Sewer. This is because the Domtar plume is diluted into relatively much more of the river flow at its ENF, as compared with the Courtaulds Storm sewer. This factor can be important when considering the possible sensitivity of mixing zone lengths, to changes in contaminant loading.

4.2.4.2 Case II: General river background concentration only:

The loading limits in this case, are derived by taking into account the existing general river background concentration using Equation 4.3. The general river background concentration used for Hg, Zn, PCBs, Phenolics and suspended solids is: 0.01, 2, 0.001, and 0.0011 ug/L, respectively. These values are based upon limited measurements, [10,14].

The results are provided in Table 4.5. Benzo(a)pyrene results are not possible for this case since there are no available river background concentration measurements for this chemical.

4.2.4.3 Case III: Both general river background, and local upstream point sources concentrations, are considered:

For this particular calculation, the loading limits take into account the sum of all background concentrations, (i.e. due to both the general upstream river chemical concentration and contributions from all local upstream point sources). There are two major types of loading limit situations to be considered for Case III.

The first situation, is when chemical loading limits are to be established for one outfall only, (i.e. the chemical loadings from the local upstream point sources are assumed fixed, and not to be modified). In this situation, Equation 4.4 can be used directly to establish the loading limit for each chemical of concern.

The second situation, is when chemical loading limits are to be established for more than one outfall simultaneously, (with at least one of these outfall plumes overlapping one or more of the other plumes). This is the situation at the Cornwall MISA Pilot Site. When this occurs, the loading limits exercise will also consist of some type of "loading allocation" component. This process is visualized by rearranging Equation 4.4 as follows:

$$C_{crit} - C_{rb} = L_{3maxn} * A_n + \sum_{i=1}^{n-1} (A_{i,n} * L_i) \qquad \ldots\ 4.5$$

Since all the outfall loading rates (i.e. the "L's"), on the right-hand-side of Equation 4.5 are to be determined, there will be infinite combinations of "L's" which could satisfy this equation, at the end of the RMZ for each downstream outfall. Thus, the total allowable chemical loadings to the river so as not to exceed "C_{crit} - C_{rb}", must be distributed, or "allocated", among the local outfalls, using some formula or assumption.

Many of the factors determining which load allocation scheme should be used, will likely involve the relative efficiency of the various treatment technologies utilized by the various industries and municipalities discharging to the water body. These factors are beyond the scope of the current work, (and would likely be considered by the MOEE District Office). As a result, only two possible procedures will be illustrated at the Cornwall MISA Pilot Site.

4.2.4.3.1 Case IIIa: Loading limits allocated, based upon upstream location:

In this loading allocation procedure, Equation 4.4 is solved to determine a fixed, maximum loading limit for each outfall <u>sequentially moving in the downstream direction</u>, starting with the outfall farthest upstream. In other words, Equation 4.4 is used to determine <u>in sequence</u>, the maximum loading limit for Outfall 1,2,3,4,...,N; using the numbering system employed for the Equations, (see the definitions for Eq. 4.1).

This load allocation procedure, in effect gives decreasing preference to the outfalls sequentially located in the downstream direction. In fact, depending upon the relative locations of upstream outfalls, and the magnitude of their allocated chemical loads, a given downstream outfall may in effect be prohibited from discharging any chemical loads, under this load allocation scheme. For this reason, it is inherently "unfair" to the downstream outfalls. However, in cases where this "unfairness" is negligible (again depending upon the locations of upstream outfalls and their chemical loads), this load allocation procedure may be favourable to others which are likely to be more cumbersome to use.

The results of applying this load allocation procedure to the 5 outfalls involved in the current study, are provided in Table 4.6, for a RMZ length equal to the near field mixing zone, ENF.

4.2.4.3.2 Case IIIb: Loading limits, based upon an "equal" allocation:

Under this load allocation scheme, in order to satisfy the criterion at the outfall farthest downstream, (which is assumed to receive the largest total impact from upstream local point sources), the loading from all outfalls, (regardless of their upstream-downstream location), are reduced by the same <u>fraction</u>, with respect to the loadings derived to meet only the general river background, (i.e. as found from Eq. 4.3). This may result in allocated loads at some of the

Table 4.4 **Maximum allowable, net loading rates assuming NO background concentrations; " CASE I ".**

SOURCE	Parameter	MAXIMUM NET LOADING RATE (kg/day), so as not to exceed the criterion at downstream distances (m), of:			
		ENF	200	500	1,000
Domtar/CIL/ Cornwall Chem. Diffuser	Hg	3.278689	4.494382	4.842615	5.747126
	Zn	491.8033	674.1573	726.3923	862.069
	PCBs	0.016393	0.022472	0.024213	0.028736
	BAP	0.000984	0.001348	0.001453	0.001724
	Phenol	16.39344	22.47191	24.21308	28.73563
	SS	16229.51	22247.19	23970.94	28448.28
Courtaulds – Viscose/Sulphide Diffuser	Hg	1.491424	4.310345	5.154639	6.60066
	Zn	223.7136	646.5517	773.1959	990.099
	PCBs	0.007457	0.021552	0.025773	0.033003
	BAP	0.000447	0.001293	0.001546	0.00198
	Phenol	7.457122	21.55172	25.7732	33.0033
	SS	7382.55	21336.21	25515.46	32673.27
Courtaulds – Acid Diffuser	Hg	1.357773	4.819277	6.097561	7.434944
	Zn	203.666	722.8916	914.6341	1115.242
	PCBs	0.006789	0.024096	0.030488	0.037175
	BAP	0.000407	0.001446	0.001829	0.00223
	Phenol	6.788866	24.09639	30.4878	37.17472
	SS	6720.978	23855.42	30182.93	36802.97
Courtaulds – Storm Outfall	Hg	0.036364	0.208986	0.267738	0.383142
	Zn	5.454545	31.34796	40.16064	57.47126
	PCBs	0.000182	0.001045	0.001339	0.001916
	BAP	0.000011	0.000063	0.00008	0.000115
	Phenol	0.181818	1.044932	1.338688	1.915709
	SS	180	1034.483	1325.301	1896.552
Cornwall WPCP Diffuser	Hg	0.440044	1.19976	1.932367	3.552398
	Zn	66.0066	179.964	289.8551	532.8597
	PCBs	0.0022	0.005999	0.009662	0.017762
	BAP	0.000132	0.00036	0.00058	0.001066
	Phenol	2.20022	5.9988	9.661836	17.76199
	SS	2178.218	5938.812	9565.217	17584.37

Table 4.5 Maximum allowable, net loading rates accounting for general river background concentrations, only; " CASE II ".

SOURCE	Parameter	Criterion Conc. [mg/L]	Average River Backgr'd Conc. [mg/L]	'Net' Criterion Conc. [mg/L]	MAXIMUM NET LOADING RATE (kg/day) so as not to exceed the 'NET' criterion at downstream distances (m), of:			
					ENF	200	500	1000
Domtar/CIL/ Cornwall Chem. Diffuser	Hg	0.0002	0.00001	0.00019	3.114754	4.269663	4.600484	5.45977
	Zn	0.03	0.002	0.028	459.0164	629.2135	677.9661	804.5977
	PCBs	1.0E−06	1.00E−06	0	0	0	0	0
	BAP	6.0E−08	0	6.0E−08	0.000984	0.001348	0.001453	0.001724
	Phenol	0.001	1.10E−06	0.000999	16.37541	22.44719	24.18644	28.70402
	SS	0.99	0.9	0.09	1475.41	2022.472	2179.177	2586.207
Courtaulds – Viscose/Sulphide Diffuser	Hg	0.0002	0.00001	0.00019	1.416853	4.094828	4.896907	6.270627
	Zn	0.03	0.002	0.028	208.7994	603.4483	721.6495	924.0924
	PCBs	1.0E−06	1.00E−06	0	0	0	0	0
	BAP	6.0E−08	0	6.0E−08	0.000447	0.001293	0.001546	0.00198
	Phenol	0.001	1.10E−06	0.000999	7.448919	21.52802	25.74485	32.967
	SS	0.99	0.9	0.09	671.1409	1939.655	2319.588	2970.297
Courtaulds – Acid Diffuser	Hg	0.0002	0.00001	0.00019	1.289885	4.578313	5.792683	7.063197
	Zn	0.03	0.002	0.028	190.0883	674.6988	853.6585	1040.892
	PCBs	1.0E−06	1.00E−06	0	0	0	0	0
	BAP	6.0E−08	0	6.0E−08	0.000407	0.001446	0.001829	0.00223
	Phenol	0.001	1.10E−06	0.000999	6.781399	24.06988	30.45427	37.13383
	SS	0.99	0.9	0.09	610.998	2168.675	2743.902	3345.725
Courtaulds – Storm Outfall	Hg	0.0002	0.00001	0.00019	0.034545	0.198537	0.254351	0.363985
	Zn	0.03	0.002	0.028	5.090909	29.2581	37.48327	53.63985
	PCBs	1.0E−06	1.00E−06	0	0	0	0	0
	BAP	6.0E−08	0	6.0E−08	0.000011	0.000063	0.00008	0.000115
	Phenol	0.001	1.10E−06	0.000999	0.181618	1.043783	1.337216	1.913602
	SS	0.99	0.9	0.09	16.36364	94.04389	120.4819	172.4138
Cornwall WPCP Diffuser	Hg	0.0002	0.00001	0.00019	0.418042	1.139772	1.835749	3.374778
	Zn	0.03	0.002	0.028	61.60616	167.9664	270.5314	497.3357
	PCBs	1.0E−06	1.00E−06	0	0	0	0	0
	BAP	6.0E−08	0	6.0E−08	0.000132	0.00036	0.00058	0.001066
	Phenol	0.001	1.10E−06	0.000999	2.1978	5.992202	9.651208	17.74245
	SS	0.99	0.9	0.09	198.0198	539.892	869.5652	1598.579

Table 4.6 Maximum allowable, net loading rates, accounting for both general river background and local point source impacts. Loads allocated using "upstream priority"; " CASE IIIa ".

SOURCE	Parameter	Criterion Conc.	Average River Backgr'd Conc.	Concentrations [ug/L], due to allocated loads discharged from upstream point source:				'Net' Criterion Conc.	Maximum net loading rate, so as not to exceed the 'net' criterion, at the ENF
		[mg/L]	[mg/L]	I.	II.	III.	IV.	[mg/L]	[kg/day]
I. Domtar/CIL/ Cornwall Chem. Diffuser	Hg	0.0002	0.00001					0.00019	3.114754
	Zn	0.03	0.002					0.028	459.0164
	PCBs	1.0E−06	1.00E−06					0	0
	BAP	6.0E−08	0					6.0E−08	0.000984
	Phenol	0.001	1.10E−06					0.000999	16.37541
	SS	0.99	0.9					0.09	1475.41
II. Courtaulds – Viscose/Sulphide Diffuser	Hg	0.0002	0.00001	0.021492				0.000169	1.256586
	Zn	0.03	0.002	3.167213				0.024833	185.1811
	PCBs	1.0E−06	1.00E−06	0				0	0
	BAP	6.0E−08	0	6.8E−06				5.3E−08	0.000397
	Phenol	0.001	1.10E−06	0.11299				0.000886	6.606336
	SS	0.99	0.9	10.18033				0.07982	595.225
III. Courtaulds – Acid Diffuser	Hg	0.0002	0.00001	0.021492				0.000169	1.14398
	Zn	0.03	0.002	3.167213				0.024833	168.5865
	PCBs	1.0E−06	1.00E−06	0				0	0
	BAP	6.0E−08	0	6.8E−06				5.3E−08	0.000361
	Phenol	0.001	1.10E−06	0.11299				0.000886	6.014322
	SS	0.99	0.9	10.18033				0.07982	541.8851
IV. Courtaulds – Storm Outfall	Hg	0.0002	0.00001	0.04018				0.00015	0.02724
	Zn	0.03	0.002	5.921311				0.022079	4.014307
	PCBs	1.0E−06	1.00E−06	0				0	0
	BAP	6.0E−08	0	0.000013				4.7E−08	8.6E−06
	Phenol	0.001	1.10E−06	0.211243				0.000788	0.14321
	SS	0.99	0.9	19.03279				0.070967	12.90313
V. Cornwall WPCP Diffuser	Hg	0.0002	0.00001	0.018066	0.012692	0.011554	0.000104	0.000148	0.32472
	Zn	0.03	0.002	2.662295	1.870329	1.702723	0.015254	0.021749	47.85346
	PCBs	1.0E−06	1.00E−06	0	0	0	0	0	0
	BAP	6.0E−08	0	5.7E−06	4.0E−06	3.6E−06	3.3E−08	4.7E−08	0.000103
	Phenol	0.001	1.10E−06	0.094977	0.066724	0.060745	0.000544	0.000776	1.707172
	SS	0.99	0.9	8.557377	6.011772	5.473039	0.049032	0.069909	153.8147

upstream outfalls, below those which would be obtained from the previous scheme, (i.e. as obtained from Equation 4.4), whereas the allocated loads toward the downstream end, would tend to be larger than obtained from Eq. 4.4.

In order to determine the loading limits for this allocation scheme, Equation 4.4 is modified by adding a "concentration reduction term", "CRT", to the right hand side of the equations, for each upstream outfall. Mathematically, this is described as follows:

$$M_i * A_i = C_{crit} - C_{rb} - \left(\sum_{j=1}^{i-1} (A_{j,i} * M_j) + CRT_i \right) \quad \ldots \; 4.6$$

where: i = *1, N*

N = *the total number of "local" outfalls, for which loads are to be allocated.*

M_i, M_j = *the largest loading permitted from outfall "i" or "j", (e.g. in kg/day).*

CRT_i = *the concentration reduction term, (e.g. in ug/L), at the end of the RMZ of outfall "i".*

C_{rb}; C_{crit}; A_i; A_j,*i: are as defined previously.*

The "concentration reduction term", is different for all outfalls. However, its value is set to zero, for the one outfall, called "n_{max}", which receives the largest impact from local upstream point sources, (i.e. for the outfall whose summation of "A_{in}* L_i" from Eq. 4.4 is the largest). This is usually the outfall farthest downstream, "N". By meeting this condition, all "CRT_i" values will be equal to or greater than zero, which of course must occur for application purposes. This condition is summarized mathematically by the following:

$$CRT_i > 0 \quad ; \quad for \;\; i = 1, N-1; \quad \ldots \; 4.7a$$

and

$$CRT_N = 0 \quad ; \quad for \; i = N. \quad \ldots \; 4.7b$$

The "equal" load allocation means that all "right-hand-sides" (and therefore all "left-hand-sides") of Equation 4.6 written out for each of the outfalls ("N" equations in total), must be equal to each other. This then leads to the following two equations, which can be used to solve for the allocated loads for all outfalls:

$$M_1 = \frac{C_{crit} - C_{rb}}{A_1 + \sum_{i=1}^{nmax-1} \left(A_{i,nmax} * \frac{A_1}{A_i} \right)} \qquad \ldots\ 4.8$$

$$M_i = \left(\frac{A_1}{A_i} \right) * M_1 \qquad \ldots\ 4.9$$

Equations 4.6 through 4.9, where written out to solve for the allocated loads, for the 5 Cornwall MISA outfalls. The results are summarized in Table 4.7, for RMZ lengths set equal to the ENF.

4.2.4.4 Comparison of the Loading Limits obtained using the different methods:

The loading limits obtained using the 3 general cases, for mixing zone lengths equivalent to the "ENFs", are summarized and compared in Table 4.8.

The differences in loading limits between Cases I and II, directly reflect the significance of considering the general river background concentration for a given chemical. The general river background concentration used for Hg, Zn, PCBs, Phenolics and suspended solids; represents about: 5, 7, 100, 0.1 and 91 %, of the respective criterion value used in this assessment. Thus, the relative impact of considering the general river background concentration in the loading limits exercise, is "nil" for Phenol; "small" for Zn and Hg; and "prohibitive" for PCBs, (i.e. no PCBs can be discharged, since the general river background concentration already equals its criterion). In fact, the actual allocated loads for Case II, are equivalent to those of Case I reduced by the above percentages. It is clear that the selection of general river background concentrations is critical, especially for PCBs.

The difference in loading limits between Cases II and III, is due to the significance of local upstream point source impacts. It can be seen that the loading limits for Case IIIa, as compared with those for Case II, are reduced in proportion by an increasing amount, (as indicated by lowering Case IIIa to Case II loading limit ratios), the farther downstream the outfall is located. This reduction ranges up to about 22 % for the Cornwall WPCP Diffuser.

For Case IIIb, (the "equally shared" load allocation), the effects of the local upstream point source impacts, in terms of creating additional loading limit reductions, is shared equally in

Table 4.7 Maximum allowable, net loading rates, accounting for both general river background and local point source impacts. Using an "equal sharing" load allocation; " CASE IIIb ".

SOURCE	Parameter	Criterion Conc. [mg/L]	Average River Backgr'd Conc. [mg/L]	Concentrations [ug/L], due to allocated loads discharged from upstream point source: I.	II.	III.	IV.	Conc. Reduction Amount [ug/L]	'Net' ENF Criterion Conc. [mg/L]	Maximum net loading rate, so as not to exceed the 'net' criterion, at the ENF [kg/day]
I. Domtar/CIL/ Cornwall Chem. Diffuser	Hg	0.0002	0.00001					0.036732	0.000153	2.512593
	Zn	0.03	0.002					5.413113	0.022587	370.2768
	PCBs	1.0E−06	1.00E−06					0	0	0
	BAP	6.0E−08	0					0.000012	4.8E−08	0.000793
	Phenol	0.001	1.10E−06					0.193113	0.000806	13.20963
	SS	0.99	0.9					17.39929	0.072601	1190.176
II. Courtaulds – Viscose/Sulphide Diffuser	Hg	0.0002	0.00001	0.017337				0.019395	0.000153	1.142939
	Zn	0.03	0.002	2.55491				2.858203	0.022587	168.4332
	PCBs	1.0E−06	1.00E−06	0				0	0	0
	BAP	6.0E−08	0	5.5E−06				6.1E−06	4.8E−08	0.000361
	Phenol	0.001	1.10E−06	0.091146				0.101966	0.000806	6.008853
	SS	0.99	0.9	8.212211				9.187082	0.072601	541.3923
III. Courtaulds – Acid Diffuser	Hg	0.0002	0.00001	0.017337				0.019395	0.000153	1.040517
	Zn	0.03	0.002	2.55491				2.858203	0.022587	153.3394
	PCBs	1.0E−06	1.00E−06	0				0	0	0
	BAP	6.0E−08	0	5.5E−06				6.1E−06	4.8E−08	0.000329
	Phenol	0.001	1.10E−06	0.091146				0.101966	0.000806	5.470381
	SS	0.99	0.9	8.212211				9.187082	0.072601	492.8765
IV. Courtaulds – Storm Outfall	Hg	0.0002	0.00001	0.032412				0.004319	0.000153	0.027867
	Zn	0.03	0.002	4.776571				0.636542	0.022587	4.106707
	PCBs	1.0E−06	1.00E−06	0				0	0	0
	BAP	6.0E−08	0	0.00001				1.4E−06	4.8E−08	8.8E−06
	Phenol	0.001	1.10E−06	0.170404				0.022709	0.000806	0.146507
	SS	0.99	0.9	15.35326				74.64674	0.072601	13.20013
V. Cornwall WPCP Diffuser	Hg	0.0002	0.00001	0.014573	0.011544	0.010509	0.000106	1.4E−20	0.000153	0.337224
	Zn	0.03	0.002	2.147606	1.701175	1.548727	0.015605	1.7E−18	0.022587	49.69612
	PCBs	1.0E−06	1.00E−06	0	0	0	0	0	0	0
	BAP	6.0E−08	0	4.6E−06	3.6E−06	3.3E−06	3.3E−08	6.6E−24	4.8E−08	0.000106
	Phenol	0.001	1.10E−06	0.076616	0.060689	0.055251	0.000557	1.1E−19	0.000806	1.772909
	SS	0.99	0.9	6.903018	5.468062	4.978053	0.05016	6.9E−18	0.072601	159.7375

Table 4.8 Comparison of water-column, dilution based, net effluent loading limits for all cases.

SOURCE	Parameter	LOADING LIMITS [Kg/day], BASED ON: No Backgr'd Conc. Method [I]	River Backgr'd Conc. Only Method [II]	River & point source backgr'd concentrations, based on : Upstream Priority Method [IIIa]	Equal Sharing Method [IIIb]	Ratio of loading limits based on various methods : meth [II] / meth [I]	meth [IIIa] / meth [II]	meth [IIIb] / meth [II]
Domtar/CIL/ Cornwall Chem. Diffuser	Hg	3.278689	3.114754	3.114754	2.512593	0.95	1	0.806675
	Zn	491.8033	459.0164	459.0164	370.2768	0.933333	1	0.806675
	PCBs	0.016393	0	0	0	0	ERR	ERR
	BAP	0.000984	0.000984	0.000984	0.000793	1	1	0.806675
	Phenol	16.39344	16.37541	16.37541	13.20963	0.9989	1	0.806675
	SS	16229.51	1475.41	1475.41	1190.176	0.090909	1	0.806675
Courtaulds – Viscose/Sulphide Diffuser	Hg	1.491424	1.416853	1.256586	1.142939	0.95	0.886885	0.806675
	Zn	223.7136	208.7994	185.1811	168.4332	0.933333	0.886885	0.806675
	PCBs	0.007457	0	0	0	0	ERR	ERR
	BAP	0.000447	0.000447	0.000397	0.000361	1	0.886885	0.806675
	Phenol	7.457122	7.448919	6.606336	6.008853	0.9989	0.886885	0.806675
	SS	7382.55	671.1409	595.225	541.3923	0.090909	0.886885	0.806675
Courtaulds – Acid Diffuser	Hg	1.357773	1.289885	1.14398	1.040517	0.95	0.886885	0.806675
	Zn	203.666	190.0883	168.5865	153.3394	0.933333	0.886885	0.806675
	PCBs	0.006789	0	0	0	0	ERR	ERR
	BAP	0.000407	0.000407	0.000361	0.000329	1	0.886885	0.806675
	Phenol	6.788866	6.781399	6.014322	5.470381	0.9989	0.886885	0.806675
	SS	6720.978	610.998	541.8851	492.8765	0.090909	0.886885	0.806675
Courtaulds – Storm Outfall	Hg	0.036364	0.034545	0.02724	0.027867	0.95	0.788525	0.806675
	Zn	5.454545	5.090909	4.014307	4.106707	0.933333	0.788525	0.806675
	PCBs	0.000182	0	0	0	0	ERR	ERR
	BAP	0.000011	0.000011	8.6E-06	8.8E-06	1	0.788525	0.806675
	Phenol	0.181818	0.181618	0.14321	0.146507	0.9989	0.788525	0.806675
	SS	180	16.36364	12.90313	13.20013	0.090909	0.788525	0.806675
Cornwall WPCP Diffuser	Hg	0.440044	0.418042	0.32472	0.337224	0.95	0.776764	0.806675
	Zn	66.0066	61.60616	47.85346	49.69612	0.933333	0.776764	0.806675
	PCBs	0.0022	0	0	0	0	ERR	ERR
	BAP	0.000132	0.000132	0.000103	0.000106	1	0.776764	0.806675
	Phenol	2.20022	2.1978	1.707172	1.772909	0.9989	0.776764	0.806675
	SS	2178.218	198.0198	153.8147	159.7375	0.090909	0.776764	0.806675
Total net loads [From all point sources]	Hg	6.604294	6.274079	5.86728	5.06114			
	Zn	990.6441	924.6011	864.6517	745.8522			
	PCBs	0.033021	0	0	0			
	BAP	0.001981	0.001981	0.001853	0.001598			
	Phenol	33.02147	32.98515	30.84645	26.60828			
	SS	32691.25	2971.932	2779.238	2397.382			

proportion, among all outfalls. The additional load reduction required for Case IIIb with respect to those of Case II, turns out to be about 19 %, (i.e. as indicated by the Case IIIb to Case II loading limit ratios of about 0.81).

It is seen then that the loading limits for the 5 parameters discharged from the 5 Cornwall outfalls examined should consider the effects of background concentrations, from both the general upstream river condition and local upstream point sources.

The loading limits provided in Tables 4.4 through 4.8, represent "net" loading limits (i.e. they include only the contaminant which is added or introduced within the waste stream of the plant, and not that already existing in the raw river water upstream of the Cornwall point sources).

The "gross" loading limits, represent the total amount of contaminants, which might be discharged in the plant's final effluent. They can be obtained mathematically as follows:

$$LL_{gross} = LL_{net} + MF_{rrw} \qquad \ldots\ 4.10$$

where: LL_{gross} = *the "gross" loading limit (e.g. in kg/day);*

LL_{net} = *the "net" loading limit (e.g. in kg/day), as provided via Methods I, II or III; and*

MF_{rrw} = *the "mass flux" within the raw river water, passed through the plant (e.g. in kg/day).*

The "mass flux" term of Equation 4.10 depends upon the location of the plant's raw water intake. However, this term can be well approximated by assuming that the raw water quality is equivalent to that of the general river background. Possible degradation of the raw water supply due to the "local", upstream point sources, will not significantly alter the value calculated for "LL_{gross}", since:

i) the effluent discharge usually represents a relatively low fraction of the river channel's flow-rate, and

ii) there is a relatively high dilution between the local upstream point sources along the Cornwall waterfront.

The gross loading limits, derived from impact in the water-column, are provided in Table 4.9.

Table 4.9 Gross effluent loading limits, for all cases based upon water-column dilution.

SOURCE	Parameter	Loading due to the river backg'd conc. [kg/day]	GROSS LOADING LIMITS [Kg/day], BASED ON:			
			No Backg'd Conc. Method [I]	River Backg'd Conc. Only Method [II]	River & point source backgr'd concentrations, using : Upstream Priority Method [IIIa]	Equal Sharing Method [IIIb]
Domtar/CIL/ Cornwall Chem. Diffuser	Hg	0.001322	3.28001	3.116076	3.116076	2.513915
	Zn	0.264384	492.0677	459.2808	459.2808	370.5412
	PCBs	0.000132	0.016526	0.000132	0.000132	0.000132
	BAP	0	0.000984	0.000984	0.000984	0.000793
	Phenol	0.000145	16.39359	16.37556	16.37556	13.20977
	SS	118.9728	16348.48	1594.383	1594.383	1309.148
Courtaulds - Viscose/Sulphide Diffuser	Hg	0.000092	1.491517	1.416946	1.256679	1.143032
	Zn	0.01849	223.7321	208.8179	185.1996	168.4516
	PCBs	9.2E-06	0.007466	9.2E-06	9.2E-06	9.2E-06
	BAP	0	0.000447	0.000447	0.000397	0.000361
	Phenol	0.00001	7.457132	7.448929	6.606346	6.008863
	SS	8.32032	7390.871	679.4613	603.5453	549.7126
Courtaulds - Acid Diffuser	Hg	0.000071	1.357844	1.289955	1.14405	1.040588
	Zn	0.01417	203.6802	190.1024	168.6006	153.3535
	PCBs	7.1E-06	0.006796	7.1E-06	7.1E-06	7.1E-06
	BAP	0	0.000407	0.000407	0.000361	0.000329
	Phenol	7.8E-06	6.788874	6.781406	6.01433	5.470389
	SS	6.37632	6727.354	617.3743	548.2614	499.2528
Courtaulds - Storm Outfall	Hg	0.000054	0.036418	0.0346	0.027294	0.027921
	Zn	0.010886	5.465432	5.101795	4.025193	4.117593
	PCBs	5.4E-06	0.000187	5.4E-06	5.4E-06	5.4E-06
	BAP	0	0.000011	0.000011	8.6E-06	8.8E-06
	Phenol	6.0E-06	0.181824	0.181624	0.143216	0.146513
	SS	4.89888	184.8989	21.26252	17.80201	18.09901
Cornwall WPCP Diffuser	Hg	0.000487	0.440531	0.418529	0.325207	0.337711
	Zn	0.097459	66.10406	61.70362	47.95092	49.79358
	PCBs	0.000049	0.002249	0.000049	0.000049	0.000049
	BAP	0	0.000132	0.000132	0.000103	0.000106
	Phenol	0.000054	2.200274	2.197853	1.707226	1.772963
	SS	43.85664	2222.074	241.8764	197.6713	203.5942
Total gross loads [From all point sources]	Hg		6.606321	6.276106	5.869307	5.063167
	Zn		991.0494	925.0065	865.0571	746.2576
	PCBs		0.033224	0.000203	0.000203	0.000203
	BAP		0.001981	0.001981	0.001853	0.001598
	Phenol		33.02169	32.98537	30.84667	26.6085
	SS		32873.68	3154.357	2961.663	2579.807

4.3 Loading limits based upon bed sediment impact

4.3.1 Procedure

As discussed earlier in Section 2.3, it is possible via Eq. 2.5 to obtain a relationship between the total contaminant concentration in the water column, "C_{T1eq}", and the particulate contaminant concentration in the bed sediment, "r_2". This equation is used to convert the estimated river background and sediment criteria, (which are in particulate concentrations of ug/g), into equivalent total water column concentrations (ug/L). By doing this, it becomes possible to use the procedures derived for the water column based loading limits (i.e. as outlined in Sections 4.2.4 through 4.2.4.3), for deriving bed sediment based loading limits as well. This is accomplished by replacing "C_{rb}" and "C_{crit}", with the "C_{T1eq}" values obtained through Eq. 2.5.

4.3.2 Selection of input values for model

For the purpose of applying the sediment impact model to derive effluent loading limits, it is assumed that the model's input parameter values will be similar to those selected during the calibration process, as outlined in Section 2.3.3.

The river background concentration in bed sediment is estimated to equal .07, 50 and .017 ug/g, for Hg, Zn and PCBs, respectively. These are obtained by geometrically averaging measured values from Stations 110 through 113 of 1979 and Station 362 of 1985.

The values of all input and model calculated parameters; including: "PC_2", the dissolved and particulate fractions, and equivalent water column criterion and river background concentrations, "$C_{scriteq}$" and "C_{sbeq}"; are provided in Table 4.10, for the three contaminants that could be evaluated, (Hg, Zn and PCBs).

4.3.3 Maximum allowable loads

The same loading scenarios evaluated for the water column based loading limits, were also evaluated in the derivation of sediment based limits. These include limits derived via: "Case I" -considering no background concentrations; "Case II" - considering only general river background concentration; and "Cases III" -considering both the general river background concentration and impact due to the local upstream point source loadings. This latter scenario considered the same two "loading allocation" possibilities, "Cases IIIa and IIIb".

4.3.3.1 Case I: No background concentrations:

Equation 4.2 was used to derive the allocated loads for this case. The results are summarized in Table 4.11.

By comparing the results in Table 4.11 with those in Table 4.4 (i.e. the bed sediment based loading limits versus the water column based loading limits), it is seen that the sediment based

loading limits are: 86, 81 and 15 % lower, for Hg, Zn and PCBs, respectively. This percentage represents the amount by which the sediment criterion is lower than, in equivalent terms, its water column counterpart.

4.3.3.2 Case II: General river background concentration only:

The loading limits for this case were derived using Equation 4.3. The results are summarized in Table 4.12.

4.3.3.3 Case IIIa: Loading limits allocated, based upon upstream location:

Equation 4.4 is used to obtain the loading limits for this case, starting at the upstream point source, and moving downstream. The limits are derived for a mixing zone length equal to the ENF. The results are provided in Table 4.13.

4.3.3.4 Case IIIb: Loading limits, based upon an "equal" allocation:

Equations 4.6 through 4.9 are used to obtain the loading limits for this case. The results are summarized in Table 4.14.

4.3.4 Comparison of the loading limits obtained using the different methods

Table 4.15 provides a summary of the net, bed sediment based, loading limits obtained for all cases.

The Case II bed sediment loading limits are reduced with respect to those of Case I, by a fraction equal to the contaminant's river background to criterion concentrations. These fractions are about 0.35, 0.34 and 1.17, for Hg, Zn and PCBs, respectively. The derived loading limits for PCBs are negative because the general river background concentration exceeds the criterion used.

By comparing the bed sediment based limits of Case IIIa to Case II it is seen that the loading limits for all contaminants are reduced by about: 11, 21 and 22 %; for the two Courtaulds' diffusers, Courtaulds shore-based sewers and Cornwall WPCP, respectively. These reductions are directly due to the accumulated impact of all local upstream point sources.

Table 4.15 also shows that for load allocation Case IIIb, the derived loading limits for all point sources are reduced by about 19 %, with respect to those obtained by considering only the general river background (i.e. Case II). This is the same percentage reduction as found for Case IIIb of the water column based loading limits, (see Table 4.8). This would be expected since the relative impact of upstream point sources due to water column advective/dispersive transport is the same for both models.

The "gross" bed sediment based loading limits can be obtained by using Eq. 4.10, in a similar

fashion as described in Section 4.2.4.4. These gross loading limits are provided in Table 4.16.

4.4 Loading limits based upon biota impact

4.4.1 Procedure

Two biota impact models were examined, as discussed in Sections 2.4 and 2.5. The predicted accuracies appear approximately the same for the two models in terms of standard deviation. However, the foodweb model was used to derive biota based loading limits, for the following reasons:

i) its biota interaction assumptions are likely more realistic, particularly in terms of the benthic-pelagic links;

ii) it incorporates a more realistic chemical depuration term;

iii) it is in general, more adaptable for future benthos analysis; and

iv) it proved to be more accurate in terms of fitting predicted to measured concentrations for both (measured) biota compartments for mercury and zinc, as indicated via geometric averages of 1 (as discussed in Section 2.5.3).

The foodweb model relates the steady state concentrations of chemical within the various aquatic biota, to that within the water column and bed sediment. As a result, it can be used to determine the maximum water column concentrations which would result in chemical concentrations within various biota equal to given criteria. Further, by coupling this relationship with the procedures derived for the water column based loading limits, loading limits, based upon biota criteria, can be derived. This is accomplished by substituting the "wet-weight basis" biota criterion for "vww_i" in Eq. 2.22, and solving for the "equivalent biota criterion in the water column", "C_{1beq}" as follows:

$$C_{1beq} = \frac{biota\ criterion}{N_i * f_{L,i}} \qquad \text{... 4.11}$$

"C_{1beq}" is then used in place of "C_{crit}" in the load allocation equations (described in Section 4.2.4).

There are only biota criterion for mercury and PCBs. Therefore, biota based loading limits could only be derived for these two contaminants.

4.4.2 Selection of input values for the model

For the purpose of applying the biota impact model to derive effluent loading limits, it is

Table 4.10 Values of variables used in the sediment model.

	INPUT VARIABLES:		
wa	settling velocity	9.75E−05	m/s
kl	water−sediment diffusion coeffic't	6.10E−06	m/s
h2	sediment layer thickness	0.03	m
ws	sedimentation velocity	3.17E−12	m/s
k2	total loss rate in sediment layer	0.00E+00	1/s
m1	sediment conc. in water column	9.00E−07	kg/L
m2	sediment conc. in sediment layer	0.549	kg/L
ff	fraction of fines in sediment	0.4	
B	calibration coef. for PC2 equation		
	Mercury:	2.553	
	Zinc:	0.766	
	PCBs:	2.52	
PC1	Partition coefficient in water col.		L/kg
	Mercury:	23900	
	Zinc:	17700	
	PCBs:	176000	
por	Porosity	0.4	
	CALCULATED VARIABLES:		
PC2	Partition coefficient in sediment		L/kg
	Mercury:	2303.865	
	Zinc:	8773.062	
	PCBs:	17486.54	
fd1	fraction dissolved in water column		
	Mercury:	0.978943	
	Zinc:	0.98432	
	PCBs:	0.86326	
fd2	fraction dissolved in sediment layer		
	Mercury:	0.000316	
	Zinc:	0.000083	
	PCBs:	0.000042	
fp1	fraction, particulate in water col.		
	Mercury:	0.021057	
	Zinc:	0.01568	
	PCBs:	0.13674	
fp2	fraction, particulate in sediment		
	Mercury:	0.999684	
	Zinc:	0.999917	
	PCBs:	0.999958	
wrs	resuspension velocity	1.57E−10	m/s
Ct1esc	Equivalent sediment criterion in water col.		mg/L
	Mercury:	2.86E−05	
	Zinc:	0.005828	
	PCBs:	8.55E−07	
Csb	Background sediment adsorbed conc.		mg/kg
	Mercury:	0.07	
	Zinc:	50	
	PCBs:	0.017	
Csbewc	Background sediment − equivalent water col.		mg/L
	Mercury:	0.00001	
	Zinc:	0.002428	
	PCBs:	2.08E−07	
Cwwb	Background, whole−water concentration in river, mg/L		
	Mercury:	0.00001	
	Zinc:	0.002	
	PCBs:	1.0E−06	
Cwcb	Background, water column conc. USED for SEDIMENT MODEL, mg/L		
	Mercury:	0.00001	
	Zinc:	0.002	
	PCBs:	1.0E−06	

Table 4.11 Sediment–based, maximum allowable, net loading rates assuming NO background concentrations; " CASE I ".

SOURCE	Parameter	MAXIMUM NET LOADING RATE (kg/day), so as not to exceed the criterion at downstream distances (m), of:			
		ENF	200	500	1,000
Domtar/CIL/ Cornwall Chem. Diffuser	Hg	0.468575	0.642316	0.692083	0.821352
	Zn	95.54439	130.971	141.1188	167.4772
	PCBs	0.014024	0.019224	0.020713	0.024582
	BAP	0	0	0	0
Courtaulds – Viscose/Sulphide Diffuser	Hg	0.213147	0.616014	0.736676	0.943335
	Zn	43.46166	125.6079	150.2115	192.3501
	PCBs	0.006379	0.018437	0.022048	0.028233
	BAP	0	0	0	0
Courtaulds – Acid Diffuser	Hg	0.194046	0.688748	0.871434	1.062567
	Zn	39.56692	140.4387	177.6893	216.662
	PCBs	0.005808	0.020614	0.026081	0.031802
	BAP	0	0	0	0
Courtaulds – Storm Outfall	Hg	0.005197	0.029867	0.038264	0.054757
	Zn	1.059674	6.090081	7.802153	11.16515
	PCBs	0.000156	0.000894	0.001145	0.001639
	BAP	0	0	0	0
Cornwall WPCP Diffuser	Hg	0.062889	0.171464	0.276165	0.507692
	Zn	12.82334	34.96226	56.31119	103.5206
	PCBs	0.001882	0.005132	0.008265	0.015195
	BAP	0	0	0	0

Table 4.12 Sediment-based, maximum allowable, net loading rates accounting for general river background concentrations only; " CASE II ".

SOURCE	Parameter	Equivalent Criterion Conc. in Water Column [mg/L]	Average River Backgr'd Conc. [mg/L]	'Net' Criterion Conc. [mg/L]	MAXIMUM NET LOADING RATE (kg/day) so as not to exceed the 'NET' criterion at downstream distances (m), of: ENF	200	500	1000
Domtar/CIL/ Cornwall Chem. Diffuser	Hg	0.000029	0.00001	0.000019	0.30464	0.417597	0.449953	0.533996
	Zn	0.005828	0.002	0.003828	62.75751	86.02715	92.69269	110.006
	PCBs	8.6E-07	1.00E-06	-1.4E-07	-0.00237	-0.00325	-0.0035	-0.00415
	BAP	0	0		0	0	0	0
Courtaulds – Viscose/Sulphide Diffuser	Hg	0.000029	0.00001	0.000019	0.138576	0.400497	0.478944	0.613302
	Zn	0.005828	0.002	0.003828	28.54741	82.50448	98.66515	126.3435
	PCBs	8.6E-07	1.00E-06	-1.4E-07	-0.00108	-0.00311	-0.00373	-0.00477
	BAP	0	0		0	0	0	0
Courtaulds – Acid Diffuser	Hg	0.000029	0.00001	0.000019	0.126158	0.447784	0.566556	0.69082
	Zn	0.005828	0.002	0.003828	25.98919	92.24598	116.7137	142.3126
	PCBs	8.6E-07	1.00E-06	-1.4E-07	-0.00098	-0.00348	-0.00441	-0.00537
	BAP	0	0		0	0	0	0
Courtaulds – Storm Outfall	Hg	0.000029	0.00001	0.000019	0.003379	0.019418	0.024877	0.0356
	Zn	0.005828	0.002	0.003828	0.696038	4.000217	5.124776	7.333732
	PCBs	8.6E-07	1.00E-06	-1.4E-07	-2.6E-05	-0.00015	-0.00019	-0.00028
	BAP	0	0		0	0	0	0
Cornwall WPCP Diffuser	Hg	0.000029	0.00001	0.000019	0.040887	0.111476	0.179546	0.330072
	Zn	0.005828	0.002	0.003828	8.4229	22.96465	36.98752	67.99659
	PCBs	8.6E-07	1.00E-06	-1.4E-07	-0.00032	-0.00087	-0.0014	-0.00257
	BAP	0	0		0	0	0	0

Table 4.13 Sediment–based, maximum allowable, net loading rates, accounting for both general river background and local point source impacts. Loads allocated using "upstream priority"; " CASE IIIa ".

SOURCE	Parameter	Equivalent Criterion Conc. in Water Column [mg/L]	Average River Backgr'd Conc. [mg/L]	Concentrations [ug/L], due to allocated loads discharged from upstream point source:				'Net' Criterion Conc. [mg/L]	Maximum net loading rate, so as not to exceed the 'net' criterion, at the ENF [kg/day]
				I.	II.	III.	IV.		
I. Domtar/CIL/ Cornwall Chem. Diffuser	Hg	0.000029	0.00001					0.000019	0.30464
	Zn	0.005828	0.002					0.003828	62.75751
	PCBs	8.6E−07	1.00E−06					−1.4E−07	−0.00237
	BAP	0	0					0	0
II. Courtaulds – Viscose/Sulphide Diffuser	Hg	0.000029	0.00001	0.002102				0.000016	0.122901
	Zn	0.005828	0.002	0.433027				0.003395	25.31828
	PCBs	8.6E−07	1.00E−06	−1.6E−05				−1.3E−07	−0.00096
	BAP	0	0	0				0	0
III. Courtaulds – Acid Diffuser	Hg	0.000029	0.00001	0.002102				0.000016	0.111888
	Zn	0.005828	0.002	0.433027				0.003395	23.04943
	PCBs	8.6E−07	1.00E−06	−1.6E−05				−1.3E−07	−0.00087
	BAP	0	0	0				0	0
IV. Courtaulds – Storm Outfall	Hg	0.000029	0.00001	0.00393				0.000015	0.002664
	Zn	0.005828	0.002	0.809572				0.003019	0.548843
	PCBs	8.6E−07	1.00E−06	−3.1E−05				−1.1E−07	−2.1E−05
	BAP	0	0	0				0	0
V. Cornwall WPCP Diffuser	Hg	0.000029	0.00001	0.001767	0.001241	0.00113	0.00001	0.000014	0.031759
	Zn	0.005828	0.002	0.363994	0.255715	0.232799	0.002086	0.002974	6.542607
	PCBs	8.6E−07	1.00E−06	−1.4E−05	−9.7E−06	−8.8E−06	−7.9E−08	−1.1E−07	−0.00025
	BAP	0	0	0	0	0	0	0	0

Table 4.14 Sediment–based, maximum allowable, net loading rates, accounting for both general river background and local point source impacts. Using an "equal sharing" load allocation; " CASE IIIb ".

SOURCE	Parameter	Equivalent Criterion Conc. in Water Column [mg/L]	Average River Backgr'd Conc. [mg/L]	Concentrations [ug/L], due to allocated loads discharged from upstream point source: I.	II.	III.	IV.	Conc. Reduction Amount [ug/L]	'Net' ENF Criterion Conc. [mg/L]	Maximum net loading rate, so as not to exceed the 'net' criterion, at the ENF [kg/day]
I. Domtar/CIL/ Cornwall Chem. Diffuser	Hg	0.000029	0.00001					0.003593	0.000015	0.245745
	Zn	0.005828	0.002					0.74009	0.003088	50.62488
	PCBs	8.6E–07	1.00E–06					–2.8E–05	–1.2E–07	–0.00191
	BAP	0	0					0	0	0
II. Courtaulds – Viscose/Sulphide Diffuser	Hg	0.000029	0.00001	0.001696				0.001897	0.000015	0.111786
	Zn	0.005828	0.002	0.349312				0.390778	0.003088	23.02847
	PCBs	8.6E–07	1.00E–06	–1.3E–05				–1.5E–05	–1.2E–07	–0.00087
	BAP	0	0	0				0	0	0
III. Courtaulds – Acid Diffuser	Hg	0.000029	0.00001	0.001696				0.001897	0.000015	0.101768
	Zn	0.005828	0.002	0.349312				0.390778	0.003088	20.96482
	PCBs	8.6E–07	1.00E–06	–1.3E–05				–1.5E–05	–1.2E–07	–0.00079
	BAP	0	0	0				0	0	0
IV. Courtaulds – Storm Outfall	Hg	0.000029	0.00001	0.00317				0.000422	0.000015	0.002726
	Zn	0.005828	0.002	0.653061				0.087029	0.003088	0.561476
	PCBs	8.6E–07	1.00E–06	–2.5E–05				–3.3E–06	–1.2E–07	–2.1E–05
	BAP	0	0	0				0	0	0
V. Cornwall WPCP Diffuser	Hg	0.000029	0.00001	0.001425	0.001129	0.001028	0.00001	8.5E–22	0.000015	0.032982
	Zn	0.005828	0.002	0.293624	0.232588	0.211745	0.002134	0	0.003088	6.794539
	PCBs	8.6E–07	1.00E–06	–1.1E–05	–8.8E–06	–8.0E–06	–8.1E–08	–6.6E–24	–1.2E–07	–0.00026
	BAP	0	0	0	0	0	0	0	0	0

Table 4.15 Comparison of sediment-based, net effluent loading limits for all cases.

SOURCE	Parameter	LOADING LIMITS [Kg/day], BASED ON: No Backgr'd Conc. Method [I]	River Backgr'd Conc. Only Method [II]	River & point source backgr'd concentrations, based on: Upstream Priority Method [IIIa]	Equal Sharing Method [IIIb]	Ratio of loading limits based on various methods: meth [II] / meth [I]	meth [IIIa] / meth [II]	meth [IIIb] / meth [II]
Domtar/CIL/ Cornwall Chem. Diffuser	Hg	0.468575	0.30464	0.30464	0.245745	0.650142	1	0.806675
	Zn	95.54439	62.75751	62.75751	50.62488	0.656841	1	0.806675
	PCBs	0.014024	−0.00237	−0.00237	−0.00191	−0.16895	1	0.806675
	BAP	0	0	0	0	ERR	ERR	ERR
Courtaulds – Viscose/Sulphide Diffuser	Hg	0.213147	0.138576	0.122901	0.111786	0.650142	0.886885	0.806675
	Zn	43.46166	28.54741	25.31828	23.02847	0.656841	0.886885	0.806675
	PCBs	0.006379	−0.00108	−0.00096	−0.00087	−0.16895	0.886885	0.806675
	BAP	0	0	0	0	ERR	ERR	ERR
Courtaulds – Acid Diffuser	Hg	0.194046	0.126158	0.111888	0.101768	0.650142	0.886885	0.806675
	Zn	39.56692	25.98919	23.04943	20.96482	0.656841	0.886885	0.806675
	PCBs	0.005808	−0.00098	−0.00087	−0.00079	−0.16895	0.886885	0.806675
	BAP	0	0	0	0	ERR	ERR	ERR
Courtaulds – Storm Outfall	Hg	0.005197	0.003379	0.002664	0.002726	0.650142	0.788525	0.806675
	Zn	1.059674	0.696038	0.548843	0.561476	0.656841	0.788525	0.806675
	PCBs	0.000156	−2.6E−05	−2.1E−05	−2.1E−05	−0.16895	0.788525	0.806675
	BAP	0	0	0	0	ERR	ERR	ERR
Cornwall WPCP Diffuser	Hg	0.062889	0.040887	0.031759	0.032982	0.650142	0.776764	0.806675
	Zn	12.82334	8.4229	6.542607	6.794539	0.656841	0.776764	0.806675
	PCBs	0.001882	−0.00032	−0.00025	−0.00026	−0.16895	0.776764	0.806675
	BAP	0	0	0	0	ERR	ERR	ERR
Total net loads [From all point sources]	Hg	0.943854	0.613639	0.573852	0.495007			
	Zn	192.456	126.413	118.2167	101.9742			
	PCBs	0.028249	−0.00477	−0.00446	−0.00385			
	BAP	0	0	0	0			

Table 4.16 Gross effluent loading limits, for all cases based upon sediment impact.

SOURCE	Parameter	Loading due to the river backg'd conc.	GROSS LOADING LIMITS [Kg/day], BASED ON:			
			No Backg'd Conc.	River Backg'd Conc. Only	River & point source backgr'd concentrations, using :	
					Upstream Priority	Equal Sharing
		[kg/day]	Method [I]	Method [II]	Method [IIIa]	Method [IIIb]
Domtar/CIL/ Cornwall Chem. Diffuser	Hg	0.001322	0.469896	0.305962	0.305962	0.247067
	Zn	0.264384	95.80878	63.02189	63.02189	50.88927
	PCBs	0.000132	0.014156	−0.00224	−0.00224	−0.00178
	BAP	0	0	0	0	0
Courtaulds – Viscose/Sulphide Diffuser	Hg	0.000092	0.21324	0.138668	0.122993	0.111878
	Zn	0.01849	43.48014	28.5659	25.33677	23.04696
	PCBs	9.2E−06	0.006389	−0.00107	−0.00095	−0.00086
	BAP	0	0	0	0	0
Courtaulds – Acid Diffuser	Hg	0.000071	0.194117	0.126229	0.111958	0.101839
	Zn	0.01417	39.58109	26.00336	23.0636	20.97899
	PCBs	7.1E−06	0.005815	−0.00097	−0.00086	−0.00078
	BAP	0	0	0	0	0
Courtaulds – Storm Outfall	Hg	0.000054	0.005251	0.003433	0.002719	0.00278
	Zn	0.010886	1.070561	0.706924	0.559729	0.572362
	PCBs	5.4E−06	0.000161	−2.1E−05	−1.5E−05	−1.6E−05
	BAP	0	0	0	0	0
Cornwall WPCP Diffuser	Hg	0.000487	0.063376	0.041374	0.032247	0.03347
	Zn	0.097459	12.9208	8.520359	6.640066	6.891998
	PCBs	0.000049	0.001931	−0.00027	−0.0002	−0.00021
	BAP	0	0	0	0	0
Total gross loads [From all point sources]	Hg		0.945881	0.615666	0.575879	0.497034
	Zn		192.8614	126.8184	118.6221	102.3796
	PCBs		0.028451	−0.00457	−0.00426	−0.00365
	BAP		0	0	0	0

assumed that the model's input parameter values will be similar to those selected during the calibration process, as outlined in Section 2.5.3. The values of all input and model calculated parameters are provided in Table 4.17, for the three contaminants that could be evaluated, (Hg, Zn and PCBs).

The more restrictive (lowest) value of "C1beq" obtained via Eq. 4.11, (as obtained by applying the equation to both fish compartments in the foodweb), is applied for obtaining loading limits. For mercury, the more restrictive value was obtained by using the forage fish, whereas for PCBs, piscivorous fish provided a more restrictive value.

4.4.3 Maximum allowable loads

The same loading scenarios evaluated for the water column based loading limits, were also evaluated in the derivation of biota based limits. These include limits derived via: "Case I" - considering no background concentrations; "Case II" - considering only general river background concentration; and "Cases III" -considering both the general river background concentration and impact due to the local upstream point source loadings. This latter scenario considered the same two "loading allocation" possibilities, "Cases IIIa and IIIb".

4.4.3.1 Case I: No background concentrations:

Equation 4.2 was used to derive the allocated loads for this case. The results are summarized in Table 4.18.

By comparing the results in Table 4.18 with those in Table 4.4, (i.e. the biota based loading limits with the water column based loading limits), it is seen that the biota based loading limits are reduced about: 18 and 29 %, for Hg and PCBs, respectively; with respect to the water column based values.

4.4.3.2 Case II: General river background concentration only:

The loading limits for this case were derived using Equation 4.3. The results are summarized in Table 4.19.

4.4.3.3 Case IIIa: Loading limits allocated, based upon upstream location:

Equation 4.4 is used to obtain the loading limits for this case, for mercury, starting at the upstream point source, and moving downstream. The limits are derived for a mixing zone length equal to the ENF. The results are provided in Table 4.20.

4.4.3.4 Case IIIb: Loading limits, based upon an "equal" allocation:

The results for this case are summarized in Table 4.21. They are derived using Eqs. 4.6 through 4.9.

4.4.4 Comparison of the loading limits obtained using the different methods.

Table 4.22 provides a summary of the net, aquatic biota based, loading limits obtained for all cases.

The loading limits for Case II are reduced with respect to those for Case I by a fraction equal to the contaminant's river background to criterion concentrations. These reduction fractions are about 0.03 and 3.40 for Hg and PCBs, respectively. The PCBs reduction factor being larger than 1.0, means that no PCBs should be discharged, since the equivalent water criterion to avoid adverse biota impact, is already less than the whole-water river background concentration.

By comparing the Case IIIa to Case II results, it is seen that the loading limit for mercury is reduced by about : 11, 21 and 22 %; for the two Courtaulds' diffusers, Courtaulds Storm sewer and Cornwall WPCP, respectively. These reductions are directly due to the accumulated impact of all upstream local point sources.

Table 4.22 also shows that for load allocation Case IIIb, the derived loading limits for all point sources are reduced by about 19 %, with respect to those obtained by considering only the general river background (i.e. Case II). This is the same percentage reduction as found for Case IIIb for the water column based and bed sediment based loading limits, (see Tables 4.8 and 4.15). This would be expected since the relative impact of upstream point sources due to water column advective/dispersive transport is the same for all three models.

As expected, the loading limits become increasingly restrictive moving from Case I to II to III, since the total background concentration considered by these cases increases. Accounting for both general river and local point source background concentrations, the allocated loads must be reduced by about: 22 and 100 %, for Hg and PCBs, respectively.

The "gross", aquatic biota based loading limits can be obtained using Eq. 4.10, in a similar fashion as described in Section 4.2.4.4. The gross loading limits are provided in Table 4.23.

5. DERIVATION OF STOCHASTIC LOADING LIMITS TO ACCOUNT FOR PARAMETER UNCERTAINTY

The loading limits derived in Section 4, (as provided in Tables 4.4 through 4.8, 4.11 through 4.15 and 4.18 through 4.22), do not consider any variability in the parameters used to define them, (such as fluctuations in the: river flow and the river background concentrations; the dynamic nature of the effluent loading rates; and calibration accuracy of the models). They are set such that the various criteria are met at the end of the RMZ, under approximate long-term average conditions for all of these parameters.

If and how statistical data on the parameter variability are considered, depends not only upon the availability of this information, but also upon the definition of "compliance". Compliance,

Table 4.17 Parameters for the 5–compartment, foodweb model.

CALIBRATED VALUES:		LOG KOW	KOW	B5S	0.1	B5W	0.9
	MERCURY	5.816	6.55E+05	P5S	0.1	P51	0.9
	ZINC	4.962	9.16E+04	P35	0.5	P32	0.5
	PCBs	5.83	6.76E+05	CALPHY	1	CALSED	1

INPUT PARAMETERS

Compart. Level	W [grams]	LIP	A	BETA	GAMA	DEL	FI	AWD	AOC	AC
1	0.0002	0.023	0.1	0.2	0.2	0.01	0.036	10	2.67	0.45
2	0.01	0.05	0.3	0.2	0.2	0.01	0.036	5	2.67	0.45
3	4	0.04	0.8	0.2	0.2	0.01	0.036	4	2.67	0.45
4	313	0.045	0.8	0.2	0.2	0.01	0.036	4	2.67	0.45
5	0.0023	0.006	0.2	0.2	0.2	0.01	0.036	7	2.67	0.45

FOCW	0.15
FOCS	0.03
CO2(Kg/L)	8.50E–06
FOCB	0.4

Contaminant Fraction Bioavailable:			
	FRACCS	FRACCW	FRACRS
MERCURY	0.01	0.01	0.01
ZINC	1	1	1
PCBs	1	1	1

	Selected "K1" values:		
	Mercury	Zinc	PCBs
Comp. 1	0.0181	0.149	0
Comp. 2	0.0181	0.149	0
Comp. 3	0.0181	0.149	0
Comp. 4	0.0181	0.149	0
Comp. 5	0.0181	0.149	0

	MERCURY				ZINC				PCBs			
	Value	Eqs LKOW range		Calc's	Value	Eqs LKOW range		Calc's	Value	Eqs LKOW range		Calc's
Eq 1 :	2.032357	2	4		0.760326	2	4		2.06538	2	4	
Eq 2 :	2.2476	4	4.5	2.2476	1.3082	4	4.5	1.3082	2.263	4	4.5	2.263
Eq 3 :	0.8	4.5	6.5	0.8	0.8	4.5	6.5	0.8	0.8	4.5	6.5	0.8
Eq 4 :	1.0736	6.5	8	0.8	1.4152	6.5	8	0.8	1.068	6.5	8	0.8
Eq 5 :	0.8552	8	8.5	0.8	1.1114	8	8.5	0.8	0.851	8	8.5	0.8
Eq 6 :	0.26472	8.5	9	0.8	0.33304	8.5	9	0.8	0.2636	8.5	9	0.8
Selected Ec & ALF				0.8				0.8				0.8

(Table 4.17 continued) **Parameters for the 5–compartment, foodweb model.**

MODEL–CALCULATED PARAMETERS (Non compartment–specific):

	CT2/CT1 [total]	PCS [bioavail.]	PCWS	PCPRIM	ILOC5	G(3,5)	G(5,1)	G5S	ALF35	ALF5S	ALF51
MERCURY	3842.653	76795.51	238255.5	196865.2	7.382322	0.493988	5.548762	1.072225	0.8	0.8	0.8
ZINC	11304.58	292435.4	697250.3	612467.2	7.382322	0.074204	0.815431	0.157571	0.8	0.8	0.8
PCBs	44924.76	582884.6	3159603	2191030	7.382322	0.754455	5.913002	1.142609	0.8	0.8	0.8

MODEL–CALCULATED PARAMETERS (Compartment–specific):

A. MERCURY :

Compart. number	GROW 1/day	RESP 1/day	KU Lw/day /kglip	K 1/day	NW Lw/ kglip	IL kgl/kgl /day	G fd.ch. mult'r	BSF Kgoc/Kglip	BAF Lw/Kglip	Criterion Whole – Biota [ug/g]	Equivalent Concentration in the water–column: dissolve Chem–Frac [ug/Lw]	dissolve Chem–Tot [ug/Lw]	dis+part Chem–Tot [ug/Lt]	Selected W/C Conc for Chem–Tot [ug/Lt]
1	0.054928	0.197741	97221.77	0.166613	6.16E+05			2.58E+00	6.16E+05					
2	0.025119	0.090428	40903.2	0.080582	3.87E+05	0.354343	2.68185	8.56E+00	2.04E+06					
3	0.007579	0.027283	19282.59	0.047555	3.50E+05	0.068089	0.493988	1.48E+01	3.53E+06	0.5	0.003546	0.354585	0.362212	
4	0.003169	0.011408	7166.646	0.029048	2.22E+05	0.016196	0.40218	6.88E+00	1.64E+06	0.5	0.006774	0.677407	0.691978	
5	0.033702	0.121327	326664.9	0.517102	5.93E+05	4.244835	6.165292	1.84E+01	4.39E+06	0.5	0.018983	1.898271	1.939103	0.362

B. ZINC :

Compart. number	GROW 1/day	RESP 1/day	KU Lw/day /kglip	K 1/day	NW Lw/ kglip	IL kgl/kgl /day	G fd.ch. mult'r	BSF Kgoc/Kglip	BAF Lw/Kglip	Criterion Whole – Biota [ug/g]	Equivalent Concentration in the water–column: dissolve Chem–Frac [ug/Lw]	dissolve Chem–Tot [ug/Lw]	dis+part Chem–Tot [ug/Lt]	Selected W/C Conc for Chem–Tot [ug/Lt]
1	0.054928	0.197741	97221.77	1.210118	9.08E+04			1.30E–01	9.08E+04					
2	0.025119	0.090428	40903.2	0.595434	6.59E+04	0.354343	0.45681	1.54E–01	1.07E+05					
3	0.007579	0.027283	19282.59	0.359458	5.25E+04	0.068089	0.074204	1.17E–01	8.15E+04		0	0	0	
4	0.003169	0.011408	7166.646	0.22722	3.11E+04	0.016196	0.056239	5.12E–02	3.57E+04		0	0	0	
5	0.033702	0.121327	326664.9	3.714353	8.72E+04	4.244835	0.906035	4.06E–01	2.83E+05		0	0	0	0

C. PCBs :

Compart. number	GROW 1/day	RESP 1/day	KU Lw/day /kglip	K 1/day	NW Lw/ kglip	IL kgl/kgl /day	G fd.ch. mult'r	BSF Kgoc/Kglip	BAF Lw/Kglip	Criterion Whole – Biota [ug/g]	Equivalent Concentration in the water–column: dissolve Chem–Frac [ug/Lw]	dissolve Chem–Tot [ug/Lw]	dis+part Chem–Tot [ug/Lt]	Selected W/C Conc for Chem–Tot [ug/Lt]
1	0.054928	0.197741	97221.77	0.143802	6.35E+05			2.01E–01	6.35E+05					
2	0.025119	0.090428	40903.2	0.0605	4.78E+05	0.354343	3.310881	8.16E–01	2.58E+06					
3	0.007579	0.027283	19282.59	0.028521	5.34E+05	0.068089	0.754455	2.76E+00	8.72E+06	0.1	0.000287	0.000287	0.000332	
4	0.003169	0.011408	7166.646	0.0106	5.20E+05	0.016196	0.941008	2.76E+00	8.73E+06	0.1	0.000255	0.000255	0.000295	
5	0.033702	0.121327	326664.9	0.483173	6.32E+05	4.244835	6.570002	2.62E+00	8.27E+06	0.1	0.002014	0.002014	0.002333	0.000294

Table 4.18 Biota–based, maximum allowable, net loading rates assuming NO background concentrations; " CASE I ".

SOURCE	Parameter	MAXIMUM NET LOADING RATE (kg/day), so as not to exceed the criterion at downstream distances (m), of:			
		ENF	200	500	1,000
Domtar/CIL/ Cornwall Chem. Diffuser	Hg	5.934426	8.134831	8.765133	10.4023
	Zn	0	0	0	0
	PCBs	0.00482	0.006607	0.007119	0.008448
Courtaulds – Viscose/Sulphide Diffuser	Hg	2.699478	7.801724	9.329897	11.94719
	Zn	0	0	0	0
	PCBs	0.002192	0.006336	0.007577	0.009703
Courtaulds – Acid Diffuser	Hg	2.45757	8.722892	11.03659	13.45725
	Zn	0	0	0	0
	PCBs	0.001996	0.007084	0.008963	0.010929
Courtaulds – Storm Outfall	Hg	0.065818	0.378265	0.484605	0.693487
	Zn	0	0	0	0
	PCBs	0.000053	0.000307	0.000394	0.000563
Cornwall WPCP Diffuser	Hg	0.79648	2.171566	3.497585	6.42984
	Zn	0	0	0	0
	PCBs	0.000647	0.001764	0.002841	0.005222

Table 4.19 Biota–based, maximum allowable, net loading rates accounting for general river background concentrations, only; " CASE II ".

SOURCE	Parameter	Equivalent Criterion Conc. in Water Column [mg/L]	Average River Backgr'd Conc. [mg/L]	'Net' Criterion Conc. [mg/L]	MAXIMUM NET LOADING RATE (kg/day) so as not to exceed the 'NET' criterion at downstream distances (m), of: ENF	200	500	1000
Domtar/CIL/ Cornwall Chem. Diffuser	Hg	0.000362	0.00001	0.000352	5.770492	7.910112	8.523002	10.11494
	Zn	0	0.002	−0.002	−32.7869	−44.9438	−48.4262	−57.4713
	PCBs	2.94E−07	1.0E−06	−7.1E−07	−0.01157	−0.01587	−0.01709	−0.02029
Courtaulds – Viscose/Sulphide Diffuser	Hg	0.000362	0.00001	0.000352	2.624907	7.586207	9.072165	11.61716
	Zn	0	0.002	−0.002	−14.9142	−43.1034	−51.5464	−66.0066
	PCBs	2.94E−07	1.0E−06	−7.1E−07	−0.00526	−0.01522	−0.0182	−0.0233
Courtaulds – Acid Diffuser	Hg	0.000362	0.00001	0.000352	2.389681	8.481928	10.73171	13.0855
	Zn	0	0.002	−0.002	−13.5777	−48.1928	−60.9756	−74.3494
	PCBs	2.94E−07	1.0E−06	−7.1E−07	−0.00479	−0.01701	−0.02152	−0.02625
Courtaulds – Storm Outfall	Hg	0.000362	0.00001	0.000352	0.064	0.367816	0.471218	0.67433
	Zn	0	0.002	−0.002	−0.36364	−2.08986	−2.67738	−3.83142
	PCBs	2.94E−07	1.0E−06	−7.1E−07	−0.00013	−0.00074	−0.00095	−0.00135
Cornwall WPCP Diffuser	Hg	0.000362	0.00001	0.000352	0.774477	2.111578	3.400966	6.25222
	Zn	0	0.002	−0.002	−4.40044	−11.9976	−19.3237	−35.524
	PCBs	2.94E−07	1.0E−06	−7.1E−07	−0.00155	−0.00424	−0.00682	−0.01254

Table 4.20 Biota-based, maximum allowable, net loading rates, accounting for both general river background and local point source impacts. Loads allocated using "upstream priority"; " CASE IIIa ".

SOURCE	Parameter	Equivalent Criterion Conc. in Water Column [mg/L]	Average River Backgr'd Conc. [mg/L]	Concentrations [ug/L], due to allocated loads discharged from upstream point source:				'Net' Criterion Conc. [mg/L]	Maximum net loading rate, so as not to exceed the 'net' criterion, at the ENF [kg/day]
				I.	II.	III.	IV.		
I. Domtar/CIL/ Cornwall Chem. Diffuser	Hg	0.000362	0.00001					0.000352	5.770492
	Zn	0	0.002					−0.002	−32.7869
	PCBs	2.94E−07	1.0E−06					−7.1E−07	−0.01157
II. Courtaulds – Viscose/Sulphide Diffuser	Hg	0.000362	0.00001	0.039816				0.000312	2.327991
	Zn	0	0.002	−0.22623				−0.00177	−13.2272
	PCBs	2.94E−07	1.0E−06	−8.0E−05				−6.3E−07	−0.00467
III. Courtaulds – Acid Diffuser	Hg	0.000362	0.00001	0.039816				0.000312	2.119373
	Zn	0	0.002	−0.22623				−0.00177	−12.0419
	PCBs	2.94E−07	1.0E−06	−8.0E−05				−6.3E−07	−0.00425
IV. Courtaulds – Storm Outfall	Hg	0.000362	0.00001	0.074439				0.000278	0.050466
	Zn	0	0.002	−0.42295				−0.00158	−0.28674
	PCBs	2.94E−07	1.0E−06	−0.00015				−5.6E−07	−0.0001
V. Cornwall WPCP Diffuser	Hg	0.000362	0.00001	0.033469	0.023513	0.021406	0.000192	0.000273	0.601586
	Zn	0	0.002	−0.19016	−0.13359	−0.12162	−0.00109	−0.00155	−3.4181
	PCBs	2.94E−07	1.0E−06	−6.7E−05	−4.7E−05	−4.3E−05	−3.8E−07	−5.5E−07	−0.00121

Table 4.21 Biota–based, maximum allowable, net loading rates, accounting for both general river background and local point source impacts. Using an "equal sharing" load allocation; " CASE IIIb ".

SOURCE	Parameter	Equivalent Criterion Conc. in Water Column [mg/L]	Average River Backgr'd Conc. [mg/L]	Concentrations [ug/L], due to allocated loads discharged from upstream point source:				Conc. Reduction Amount [ug/L]	'Net' ENF Criterion Conc. [mg/L]	Maximum net loading rate, so as not to exceed the 'net' criterion, at the ENF [kg/day]
				I.	II.	III.	IV.			
I. Domtar/CIL/ Cornwall Chem. Diffuser	Hg	0.000362	0.00001					0.068051	0.000284	4.654909
	Zn	0	0.002					−0.38665	−0.00161	−26.4483
	PCBs	2.94E−07	1.0E−06					−0.00014	−5.7E−07	−0.00934
II. Courtaulds – Viscose/Sulphide Diffuser	Hg	0.000362	0.00001	0.032119				0.035932	0.000284	2.117445
	Zn	0	0.002	−0.18249				−0.20416	−0.00161	−12.0309
	PCBs	2.94E−07	1.0E−06	−6.4E−05				−7.2E−05	−5.7E−07	−0.00425
III. Courtaulds – Acid Diffuser	Hg	0.000362	0.00001	0.032119				0.035932	0.000284	1.927695
	Zn	0	0.002	−0.18249				−0.20416	−0.00161	−10.9528
	PCBs	2.94E−07	1.0E−06	−6.4E−05				−7.2E−05	−5.7E−07	−0.00387
IV. Courtaulds – Storm Outfall	Hg	0.000362	0.00001	0.060048				0.008002	0.000284	0.051627
	Zn	0	0.002	−0.34118				−0.04547	−0.00161	−0.29334
	PCBs	2.94E−07	1.0E−06	−0.00012				−1.6E−05	−5.7E−07	−0.0001
V. Cornwall WPCP Diffuser	Hg	0.000362	0.00001	0.026998	0.021386	0.01947	0.000196	0	0.000284	0.624751
	Zn	0	0.002	−0.1534	−0.12151	−0.11062	−0.00111	−1.1E−19	−0.00161	−3.54972
	PCBs	2.94E−07	1.0E−06	−5.4E−05	−4.3E−05	−3.9E−05	−3.9E−07	−5.3E−23	−5.7E−07	−0.00125

Table 4.22 **Comparison of biota-based, net effluent loading limits for all cases.**

SOURCE	Parameter	LOADING LIMITS [Kg/day], BASED ON: No Backgr'd Conc. Method [I]	River Backgr'd Conc. Only Method [II]	River & point source backgr'd concentrations, based on : Upstream Priority Method [IIIa]	Equal Sharing Method [IIIb]	Ratio of loading limits based on various methods : meth [II] / meth [I]	meth [IIIa] / meth [II]	meth [IIIb] / meth [II]
Domtar/CIL/ Cornwall Chem. Diffuser	Hg	5.934426	5.770492	5.770492	4.654909	0.972376	1	0.806675
	Zn	0	−32.7869	−32.7869	−26.4483	ERR	1	0.806675
	PCBs	0.00482	−0.01157	−0.01157	−0.00934	−2.40136	1	0.806675
Courtaulds – Viscose/Sulphide Diffuser	Hg	2.699478	2.624907	2.327991	2.117445	0.972376	0.886885	0.806675
	Zn	0	−14.9142	−13.2272	−12.0309	ERR	0.886885	0.806675
	PCBs	0.002192	−0.00526	−0.00467	−0.00425	−2.40136	0.886885	0.806675
Courtaulds – Acid Diffuser	Hg	2.45757	2.389681	2.119373	1.927695	0.972376	0.886885	0.806675
	Zn	0	−13.5777	−12.0419	−10.9528	ERR	0.886885	0.806675
	PCBs	0.001996	−0.00479	−0.00425	−0.00387	−2.40136	0.886885	0.806675
Courtaulds – Storm Outfall	Hg	0.065818	0.064	0.050466	0.051627	0.972376	0.788525	0.806675
	Zn	0	−0.36364	−0.28674	−0.29334	ERR	0.788525	0.806675
	PCBs	0.000053	−0.00013	−0.0001	−0.0001	−2.40136	0.788525	0.806675
Cornwall WPCP Diffuser	Hg	0.79648	0.774477	0.601586	0.624751	0.972376	0.776764	0.806675
	Zn	0	−4.40044	−3.4181	−3.54972	ERR	0.776764	0.806675
	PCBs	0.000647	−0.00155	−0.00121	−0.00125	−2.40136	0.776764	0.806675
Total net loads [From all point sources]	Hg	11.95377	11.62356	10.86991	9.376427			
	Zn	0	−66.0429	−61.7608	−53.2752			
	PCBs	0.009708	−0.02331	−0.0218	−0.01881			

Table 4.23 Gross effluent loading limits, for all cases based upon biota impact.

SOURCE	Parameter	Loading due to the river backg'd conc. [kg/day]	GROSS LOADING LIMITS [Kg/day], BASED ON: No Backg'd Conc. Method [I]	River Backg'd Conc. Only Method [II]	River & point source backgr'd concentrations, using : Upstream Priority Method [IIIa]	Equal Sharing Method [IIIb]
Domtar/CIL/ Cornwall Chem. Diffuser	Hg	0.001322	5.935748	5.771814	5.771814	4.656231
	Zn	0.264384	0.264384	−32.5225	−32.5225	−26.184
	PCBs	0.000132	0.004952	−0.01144	−0.01144	−0.0092
Courtaulds – Viscose/Sulphide Diffuser	Hg	0.000092	2.69957	2.624999	2.328084	2.117538
	Zn	0.01849	0.01849	−14.8958	−13.2087	−12.0125
	PCBs	9.2E−06	0.002202	−0.00526	−0.00466	−0.00424
Courtaulds – Acid Diffuser	Hg	0.000071	2.45764	2.389752	2.119444	1.927766
	Zn	0.01417	0.01417	−13.5636	−12.0277	−10.9386
	PCBs	7.1E−06	0.002003	−0.00479	−0.00424	−0.00386
Courtaulds – Storm Outfall	Hg	0.000054	0.065873	0.064054	0.05052	0.051682
	Zn	0.010886	0.010886	−0.35275	−0.27585	−0.28245
	PCBs	5.4E−06	0.000059	−0.00012	−9.6E−05	−9.8E−05
Cornwall WPCP Diffuser	Hg	0.000487	0.796967	0.774965	0.602074	0.625239
	Zn	0.097459	0.097459	−4.30298	−3.32065	−3.45226
	PCBs	0.000049	0.000696	−0.0015	−0.00116	−0.0012
Total gross loads [From all point sources]	Hg		11.9558	11.62558	10.87193	9.378454
	Zn		0.405389	−65.6375	−61.3554	−52.8698
	PCBs		0.009911	−0.02311	−0.0216	−0.0186

should involve both quantitative and temporal components. In other words, it is crucial to know whether the concentration must be at or below the criterion all of the time, on average, or some other given percentage of the time, (e.g. 95 %). Also, if compliance is for some percentage of the time, it is also likely important to stipulate the maximum continuous length of time when the concentration may exceed the criterion, and by what magnitude, for a given exceedence event, (e.g. the criterion may be exceeded by up to 10 %, for a maximum of 1 day at a time, and overall, must comply with the criterion 95 % of the time).

For the purposes of this exercise, it is assumed that compliance to a given criterion may be required for more than 50 % of the time. As such, the loading limits derived in Section 4 must be altered (i.e. lowered) to account for variability in the parameters used to derive them. A method for accounting for parameter uncertainty is documented in this section of the report. It is also applied to reveal how the derived loading limits would vary, to meet different levels of compliance.

Even if different levels of compliance are not chosen, the information obtained in this section is important to gain a better understanding of the sensitivity of the derived loading limits of Section 4, to parameter uncertainty.

5.1 Review of approaches used in the past

In reviewing two key references regarding the accommodation of parameter uncertainty to derived loading limits [16,22], two general types of approach are seen.

5.1.1 St. Clair River MISA Pilot Site method

For the St. Clair River MISA Pilot Site work [16], the general uncertainty equation used is outlined as follows:

$$\frac{C}{C_m} = \frac{L}{L_{50}} * \frac{Q_{50}}{Q} \qquad \ldots\ 5.1a$$

where: C = *the actual chemical concentration for a given load and river flow rate;*

L = *the actual effluent loading rate;*

Q = *the actual river flow rate;*

C_m = *the modelled concentration under median: loading rate, river flow rate and modelling calibration error;*

L_{50} = *the median effluent loading rate; and*

Q_{50} = *the median river flow rate.*

By making the reasonable assumption that the variances in the model calibration, river flow-rate and effluent loading rate, are random and independent, the following total variance equation is derived:

$$V_c = V_{sm} + V_Q + V_L \qquad \ldots\ 5.1b$$

where: V_c = *the total variance in the predicted concentration at the end of the mixing zone;*

V_{sm} = *the variance in the calibration error of the model (obtained by plotting the predicted versus measured data set);*

V_Q = *the variance in the river flow-rate; and*

V_L = *the variance in the effluent loading rate.*

It was found that a lognormal distribution, best fit the range in values exhibited by the parameters represented in Eq. 5.1a.

In the St. Clair MISA Pilot Site work, the contaminants of key interest were highly unique to the point sources analyzed, (i.e. the loading from the point sources far exceeded those within the upstream river background). As such, the variability of river background concentrations was not considered, (since they would not significantly alter any of the derived loading limits).

5.1.2 Lake Ontario Fate of Toxics Modelling

The modelling work conducted in support of the "Lake Ontario Toxics Management Plan" [22], involved deriving total loading limits for selected contaminants to Lake Ontario.

There was not sufficient data for model calibration. Therefore variance in model predictions, due to "total" calibration error, (the sum of: conceptual flaws in the model; neglect of phenomena of first-order importance; and uncertainty of parameter values), could not be established. However, a "Monte Carlo" approach was utilized to evaluate the effect of model parameter uncertainty, upon the predicted results from the model, in order to place some confidence limits on the recommended loading limits.

In the "Monte Carlo" method used, probability distributions were derived for all key modelling parameters, (based upon literature and/or data from similar previous field work). Several random combinations (300 in total) of these modelling parameters were formed, then the model was used to obtain 300 output results. These 300 output results were then fit to a probabilistic

distribution, in order to relate the contaminant's loading rate, to its frequency of compliance with a given criterion.

Most of the modelling parameters were best described using a lognormal distribution. As a result, the results of the stochastic analysis of the multiple model runs also tended to be lognormal in nature.

5.2 Derivation of load allocation equations to account for parameter uncertainty

The Cornwall MISA Pilot Site situation is significantly different to the two referenced studies outlined in Section 5.1, since:

i) The upstream river background concentrations of several of the contaminants of interest, are significant, in comparison with their respective concentration criteria. As a result, the procedure adopted to look at total uncertainty must consider the uncertainty introduced by variability in the upstream river background concentrations.

ii) There are multiple, overlapping point sources for which loading limits are being derived simultaneously. For any given point source, the uncertainty in the additional background concentration introduced by each of the upstream overlapping point sources, must be considered.

Since background concentrations must be considered, whether due to general river or local point sources, a general linear uncertainty equation can not be derived, as was done for the St. Clair MISA Pilot Site work. This is easily seen by comparing the general form of Eq. 5.1a with Eqs. 4.2, 4.3 and 4.4. As a result, it is not possible to derive a simple expression for total variance such as Eq. 5.1b. A "Monte Carlo" approach is more appropriate, since it will allow the estimation of the total variance via use of the actual loading limit equations of Section 4.

The general loading limit equations outlined in Section 4, were modified to account for variable parameter values. This was done by introducing "uncertainty factors" for each of the key modelling parameters utilized in the loading limit equations. These uncertainty factors are used to alter the values of the parameters, within their measured (or estimated) ranges, according to their statistical characteristics.

Three of these "uncertainty factors", deal with the calibration errors associated with the water column, bed sediment, and biota food web models. They are namely:

WCF: "The water column model, calibration error, uncertainty factor": This factor directly affects the value of the "A_i" and "$A_{i,n}$" parameters used in the loading limit equations. These factors relate effluent loading to ambient concentration in the water-column, (e.g. (ug/L) / (kg/day)), for all outfalls. Thus, the WCF provides a direct indication of the effects of calibration uncertainty of the water column impact model upon its predicted results.

SCF: "The sediment model, calibration error, uncertainty factor": This factor is used to alter the value of the "equivalent sediment criterion in the water column", (see Sections 2.3.1 and 4.3), since the accuracy of this criterion is directly proportional to the sediment model's calibration accuracy. Therefore, the SCF provides a direct indication of the effects of calibration uncertainty of the sediment impact model upon its predicted results.

BCF: "The aquatic biota model, calibration error, uncertainty factor": This factor is used to alter the value of the "equivalent aquatic biota criterion in the water column", (see Section 4.4.1), since the accuracy of this criterion is directly proportional to the aquatic biota model's calibration accuracy. Therefore the BCF provides a direct indication of the effects of calibration uncertainty of the aquatic biota impact model upon its predicted results.

The other two "uncertainty factors" deal with the values of the river flow-rate and river background contaminant concentration. They are:

RBC: "The river background concentration, uncertainty factor": This factor is used to adjust the river background concentrations used in the loading limit equations.

RFR: "The river flow-rate, uncertainty factor": This factor directly effects the value of the "A_i" and "$A_{i,j}$" parameters used in the loading limit equations, (i.e. the dilution in the water-column). These factors relate effluent loading to ambient concentration in the water-column, (e.g. (ug/L) / (kg/day)). It is assumed that these "A" values vary (inversely) proportionately to changes in the river flow-rate [15].

5.2.1 Uncertainty equations for Load Allocation Case IIIa

By incorporating the 5 "uncertainty factors", the loading limit equations are modified (from Eq. 4.4) as follows, for load allocation Case IIIa:

a) based upon the water column model:

$$L_n = \frac{C_{crit} - C_{rb} * RBC - \sum_{i=1}^{n-1} (A_{i,n} * L_i) * WCF * RFR}{A_n * WCF * RFR} \qquad \ldots\ 5.2$$

b) based upon the bed sediment model:

$$L_n = \frac{C_{crit} * SCF - C_{rb} * RBC - \sum_{i=1}^{n-1} (A_{i,n} * L_i) * RFR}{A_n * RFR} \qquad \ldots\ 5.3$$

c) based upon the biota model:

$$L_n = \frac{C_{crit} * BCF - C_{rb} * RBC - \sum_{i=1}^{n-1} (A_{i,n} * L_i) * RFR}{A_n * RFR} \qquad \dots\ 5.4$$

5.2.2 Uncertainty equations for Load Allocation Case IIIb

For load allocation Case IIIb, Eq. 4.8 is modified to describe the allocated load for the outfall farthest upstream, (outfall Number "1"), as follows:

a) based upon the water column model:

$$L_1 = \frac{C_{crit} - C_{rb} * RBC}{A_1 * WCF * RFR + \sum_{i=1}^{nmax-1} \left(A_{i,nmax} * WCF * RFR * \frac{A_1}{A_i} \right)} \qquad \dots\ 5.5$$

b) based upon the sediment model:

$$L_1 = \frac{C_{crit} * SCF - C_{rb} * RBC}{A_1 * RFR + \sum_{i=1}^{nmax-1} \left(A_{i,nmax} * RFR * \frac{A_1}{A_i} \right)} \qquad \dots\ 5.6$$

c) based upon the biota model:

$$L_1 = \frac{C_{crit} * BCF - C_{rb} * RBC}{A_1 * RFR + \sum_{i=1}^{nmax-1} \left(A_{i,nmax} * RFR * \frac{A_1}{A_i} \right)} \qquad \dots\ 5.7$$

Equation 4.9, which is used to obtain the allocated load for the other downstream outfalls (outfall Numbers "2" through "N"), is not altered, since the same uncertainty factors would exist in both the numerator and denominator.

It should be pointed out that the equations 5.2 through 5.7, do not consider variability in the

effluent loading rates (i.e. short term fluctuations with respect to the median loading rate). These were not considered since detailed (high frequency) effluent monitoring data was not available. Fluctuations in the loading rate would increase the total uncertainty, thus resulting in a greater variance in the probabilistic loading limits.

Equations 5.2 through 5.7 could be easily modified to account for uncertainty in the effluent loading rate, by introducing uncertainty factors for each of the outfalls, (i.e. each of the outfall's "L" or "A" parameters). This step would increase the number of "uncertainty factors" (from 5 to 10, in the Cornwall MISA application). This in turn, would likely require an increase in the number of Monte Carlo simulations made, in order to ascertain the stochastic nature of the load allocation results.

Equations 5.2 through 5.4, (or 5.5 through 5.7), can also be easily altered to provide the uncertainty equations for Load Allocation Cases I and II. Case I, (no background concentration consideration), is obtained by setting "C_{rb}" and the "$A_{i,n}$" parameters to zero. Case II, (general river background concentration only considered), is obtained by setting only the "$A_{i,n}$" parameters to zero.

5.3 General procedure for application of the uncertainty equations

In order to obtain stochastic loading limits, the following procedure was applied:

1) The "uncertainty equations" were incorporated into a "Monte Carlo" framework, (to permit multiple sets of input parameters and simulated output results);

2) For each of the 5 key parameters, the range of values were measured and fit to statistical distributions, based upon actual data;

3) For each parameter, multiple "uncertainty factors" were generated based upon the parameter's statistical distribution obtained in Step 2. These multiple "uncertainty factors" were then randomly ordered;

4) The "Monte Carlo" framework was used to produce multiple loading limits for each outfall by making multiple simulations (using the multiple groups of parameter "uncertainty factors" obtained in Step 3); and

5) The multiple loading limits were statistically analyzed to obtain the final probabilistic loading limits for each outfall.

These steps are elaborated upon further in report Sections 5.3.1 through 5.3.4, which follow.

5.3.1 Development of a "Monte Carlo" framework

The uncertainty loading limit equations, (i.e. Eqs. 5.2 to 5.7 and 4.9), were programmed using

the "Microsoft FORTRAN" (Version 4.1) compiler. Two programs were written, one each for loading allocation Methods 3A and 3B. A listing of the source code is provided in Appendix VII.

The user specifies the input file name containing all input parameters needed for carrying out the "Monte Carlo" simulations. These parameters include the:

- number of chemicals, outfalls and simulations to be made;
- water, sediment and biota criterion, for each chemical;
- median river background concentration for each chemical;
- median unit water column dispersion results, (i.e. all median "A" values); and
- all (randomly ordered) "uncertainty factor" data sets, for the 5 variable parameters, (i.e. "WCF", "SCF", "BCF", "RBC" and "RFR"). The total number of data sets is equal to the number of simulations to be made.

The program then calculates the loading limits for all outfalls, for each group of statistical input parameters, and saves the results in user specified output files.

5.3.2 Estimation of the parameters' statistical distributions

The statistical distributions for all parameters were estimated using the "STATGRAPHICS" (Version 4.0), software package.

5.3.2.1 Statistical distribution of the calibration results:

The statistical distributions of the calibration results for the three models, (water column, bed sediment and aquatic biota), were obtained by examining the actual pairs of predicted versus measured data points. The range of predicted/measured values were plotted, using different statistical distributions, in order to obtain an appropriate stochastic description. It was found that the predicted/measured data points were best described via a lognormal distribution.

The actual data, along with the fitted distribution for the: water column model (applicable to all parameters of concern); bed sediment model (for Hg, Zn and PCBs); and biota model (for Hg, Zn and PCBs); are plotted on Figures 5.1 through 5.7, respectively. The statistical information describing the fitted distributions are provided in Table 5.1.

5.3.2.2 River flow-rate variability:

In order to approximate the river flow-rate variability, 21 years worth of monthly-average total river flow-rates, from 1960 to 1980, were analyzed. A lognormal distribution was found to best fit the flow-rate data.

The flow-rate data, along with the fitted distribution are plotted in Figure 5.8. The statistical information describing the fitted distributions are provided in Table 5.1.

Figure 5.1 Probability plot of the

water column model calibration error.

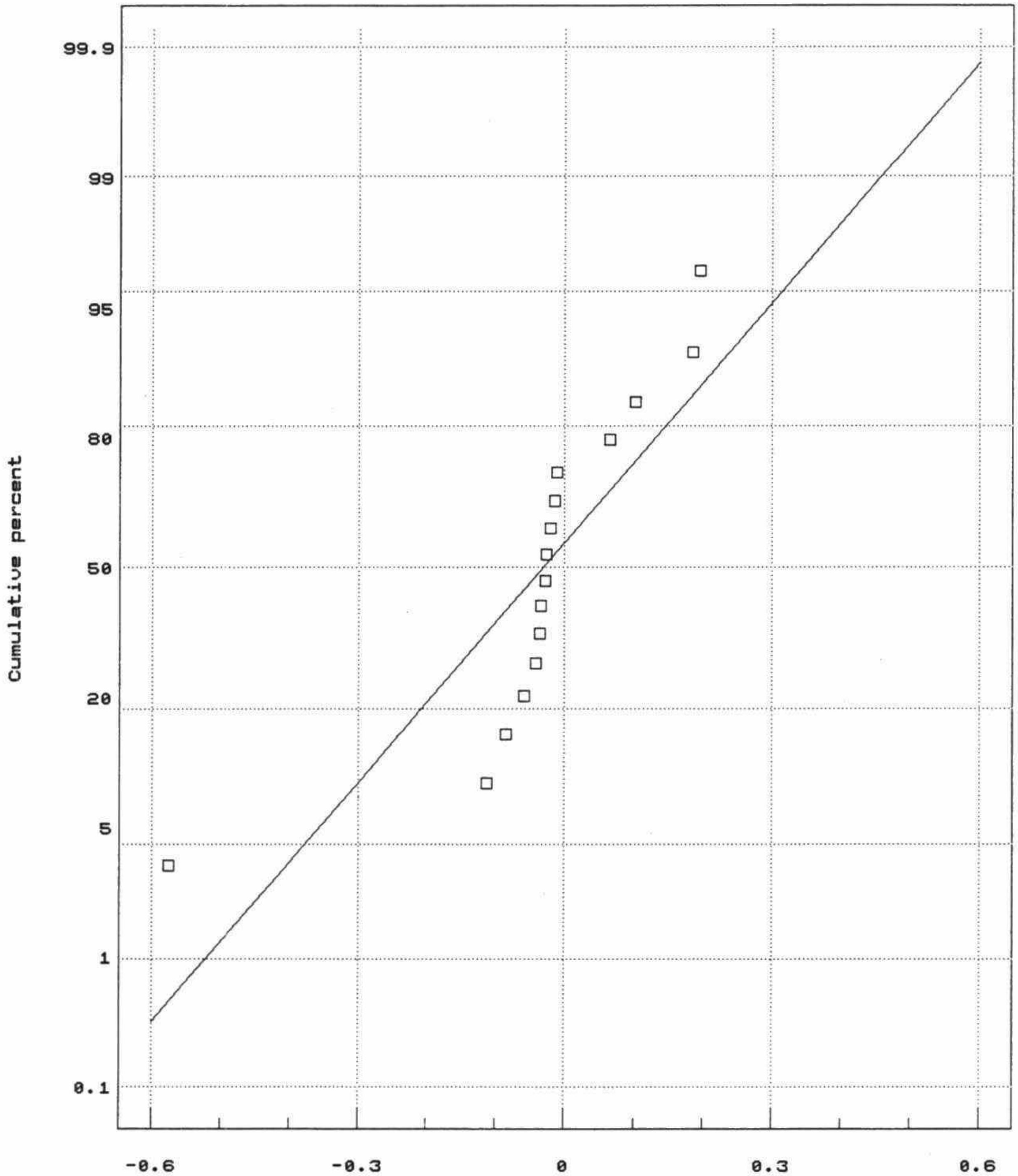


Figure 5.2 Probability plot of the Hg

sediment model calibration error.

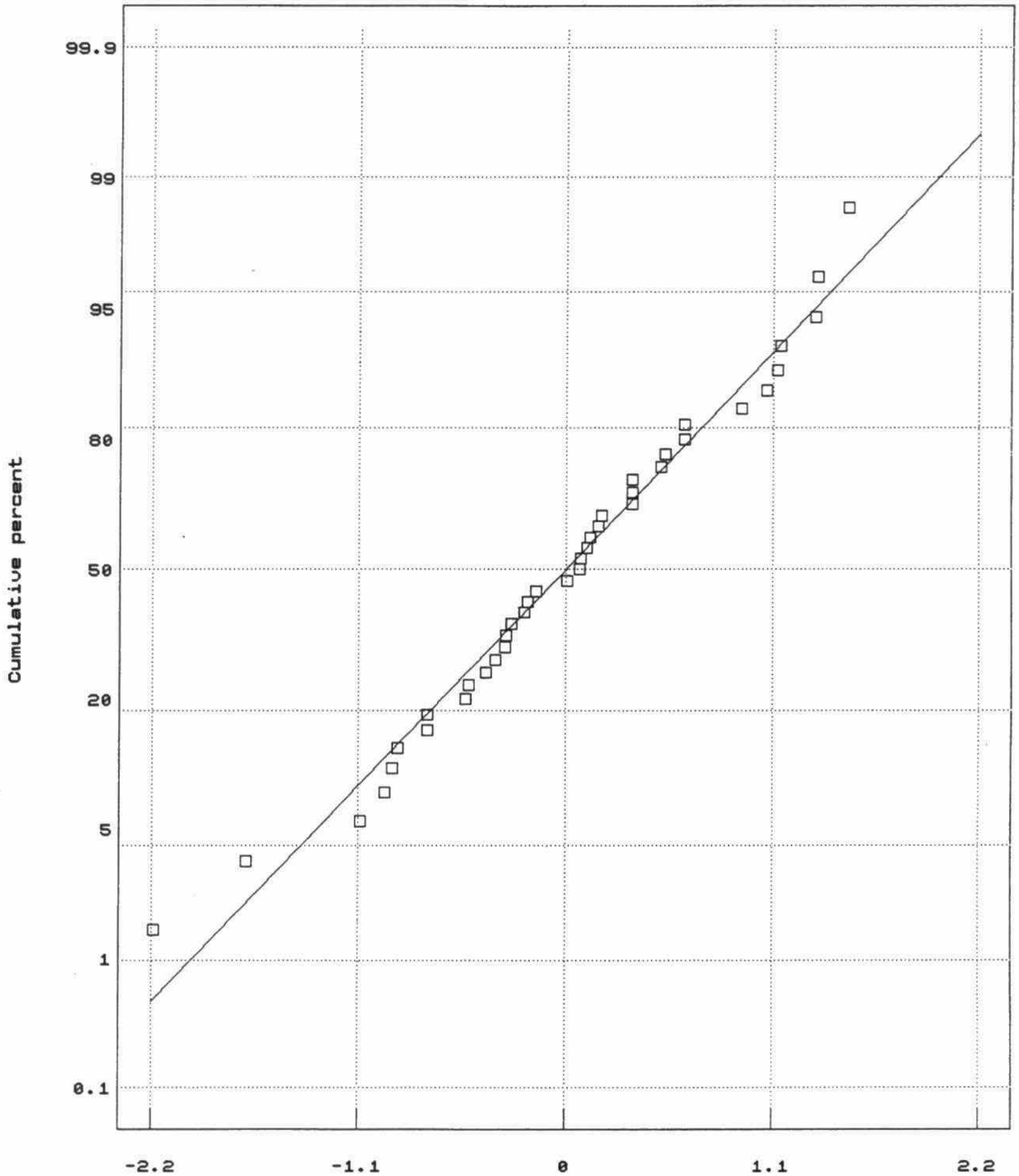


Figure 5.3 Probability plot of the Zn

sediment model calibration error.

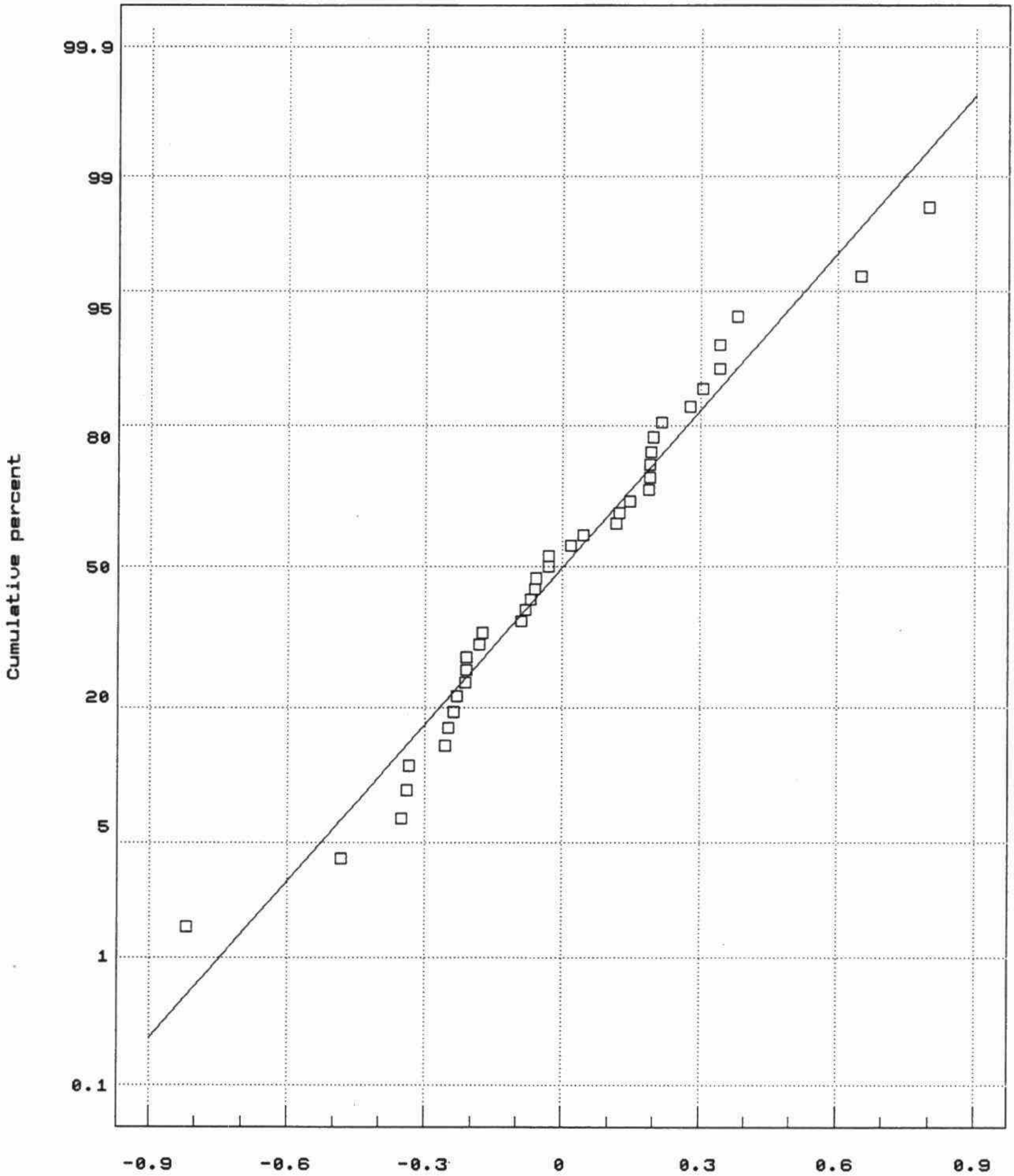


Figure 5.4 Probability plot of the PCBs

sediment model calibration error.

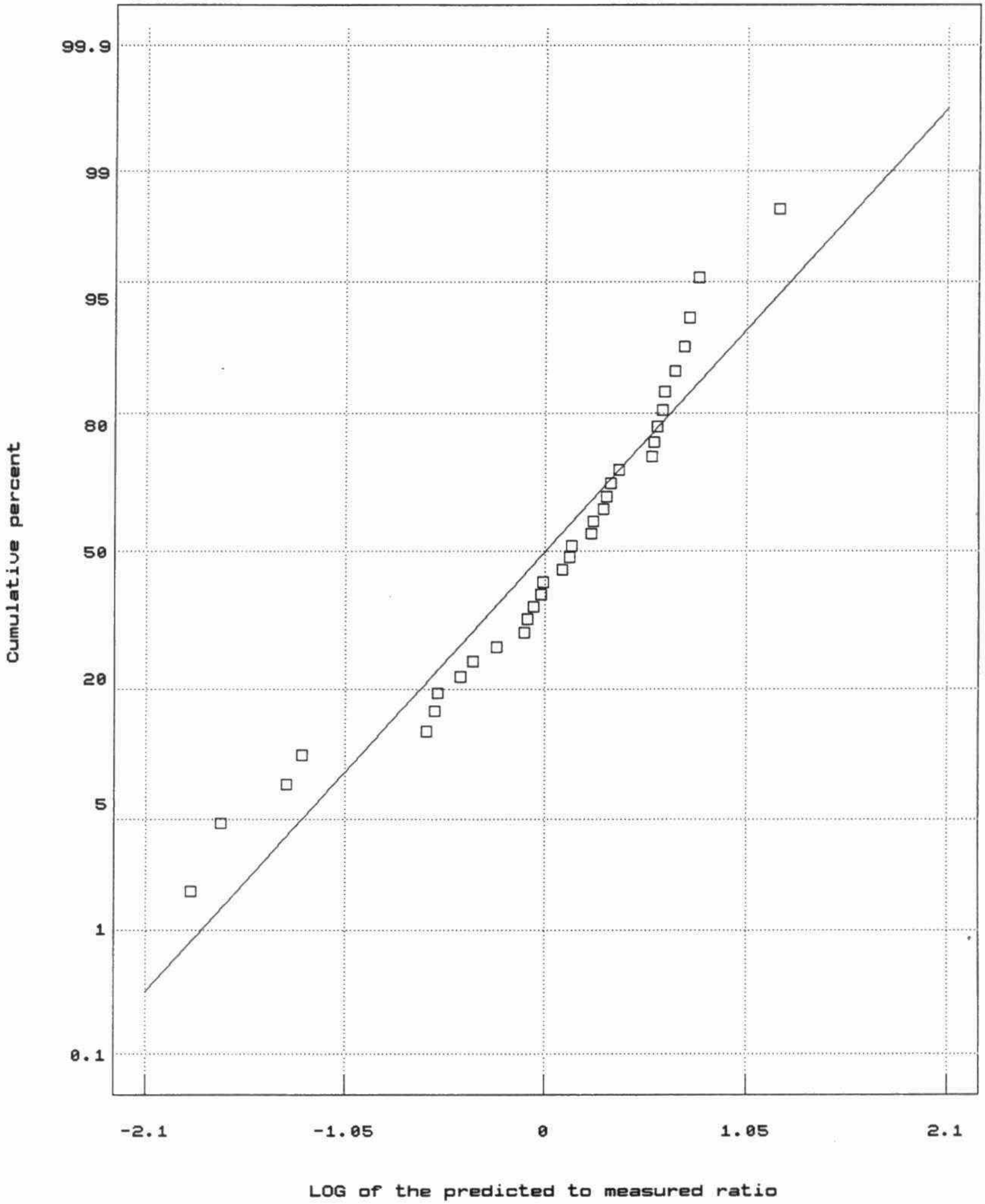


Figure 5.5 Probability plot of the Hg

biota model calibration error.

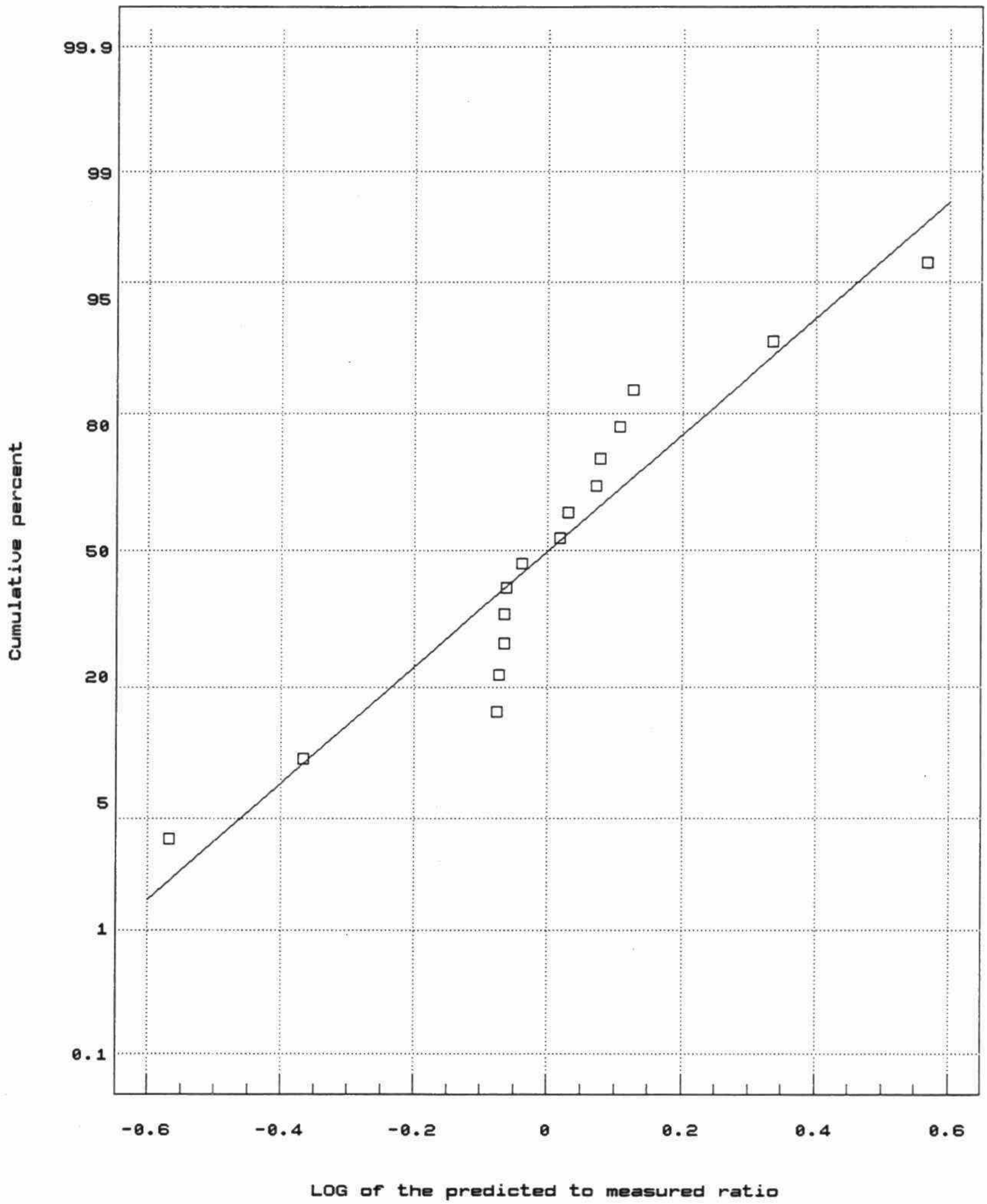


Figure 5.6 Probability plot of the Zn

biota model calibration error.

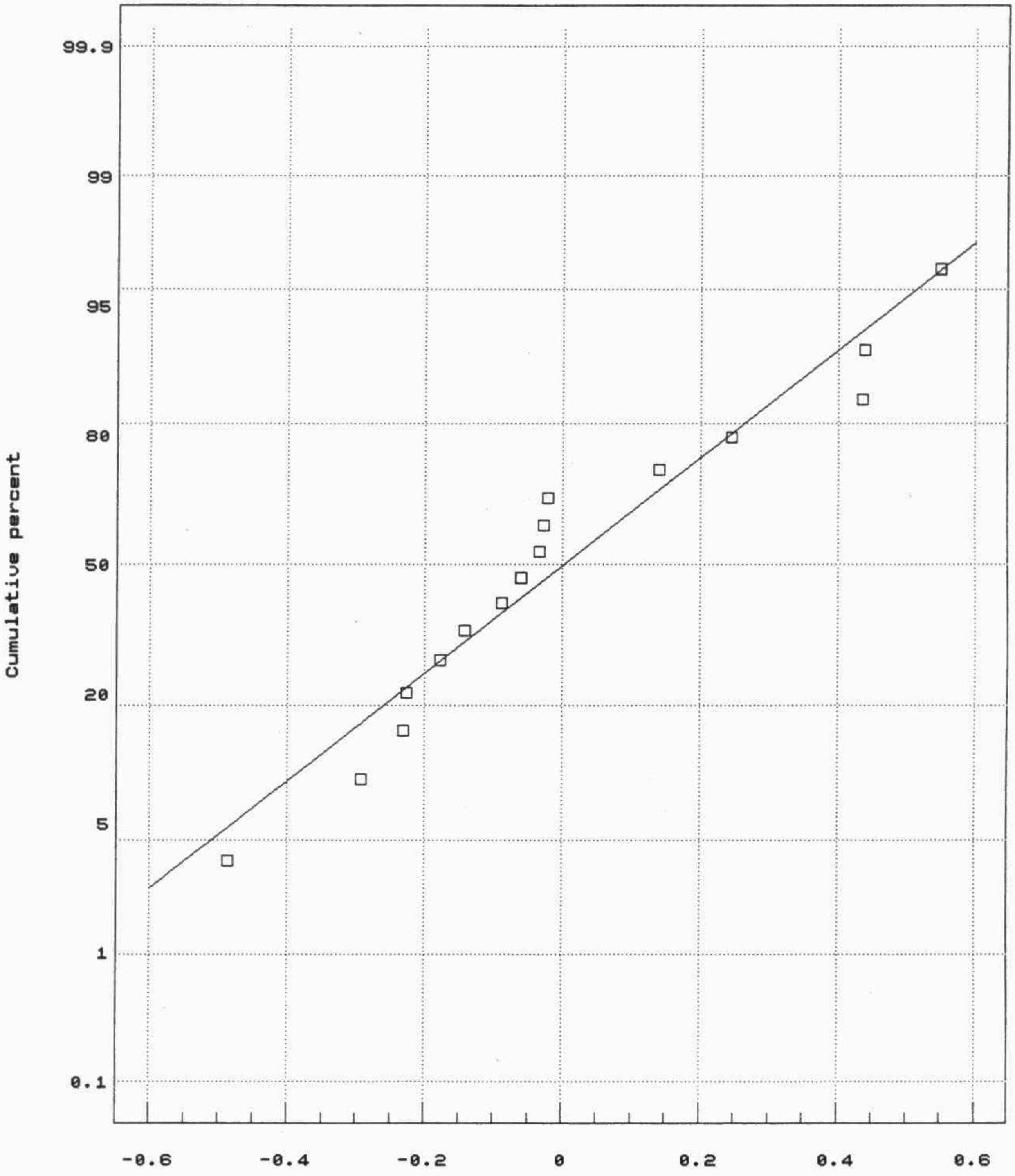


Figure 5.7 Probability plot of the PCBs

biota model calibration error.

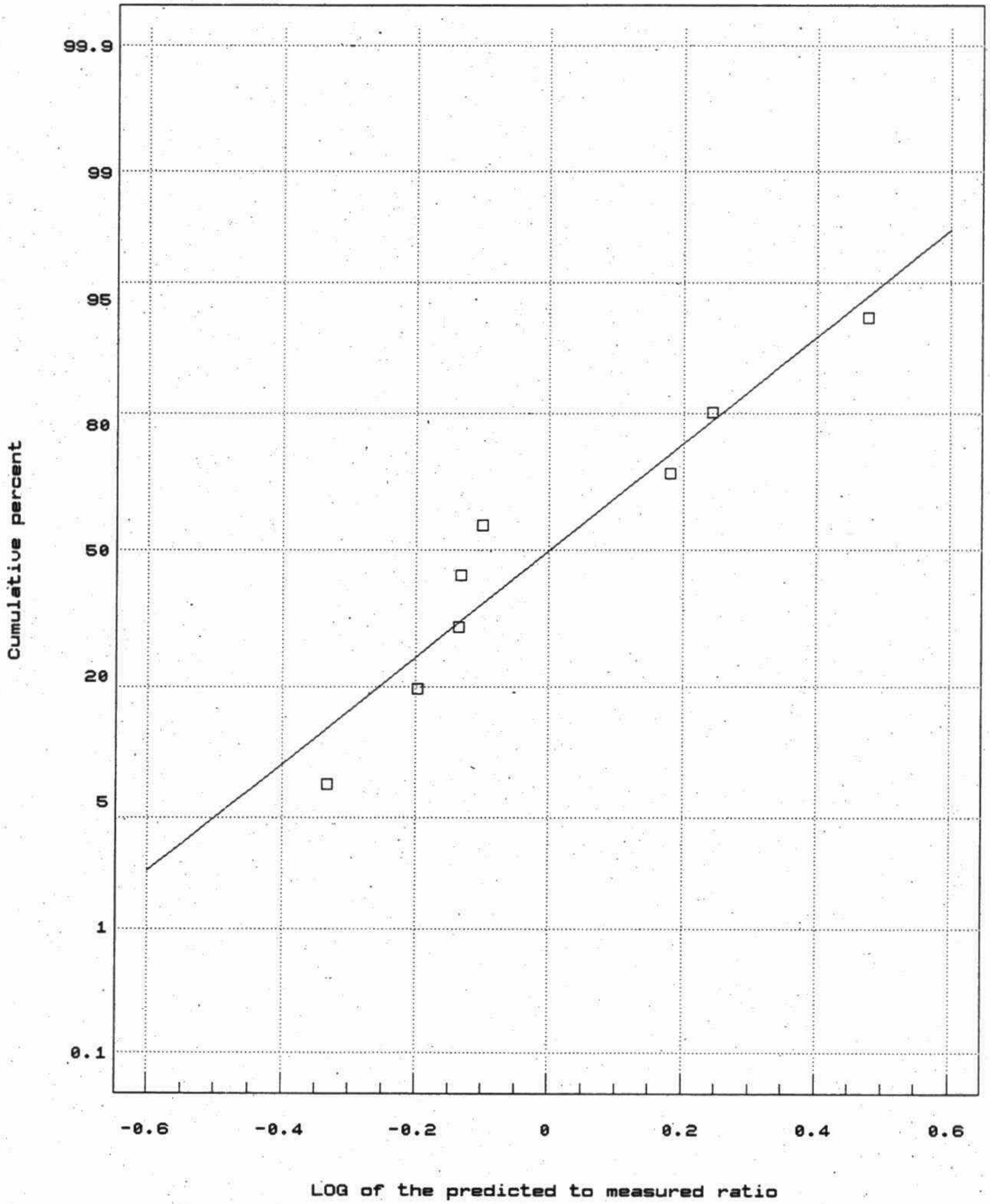
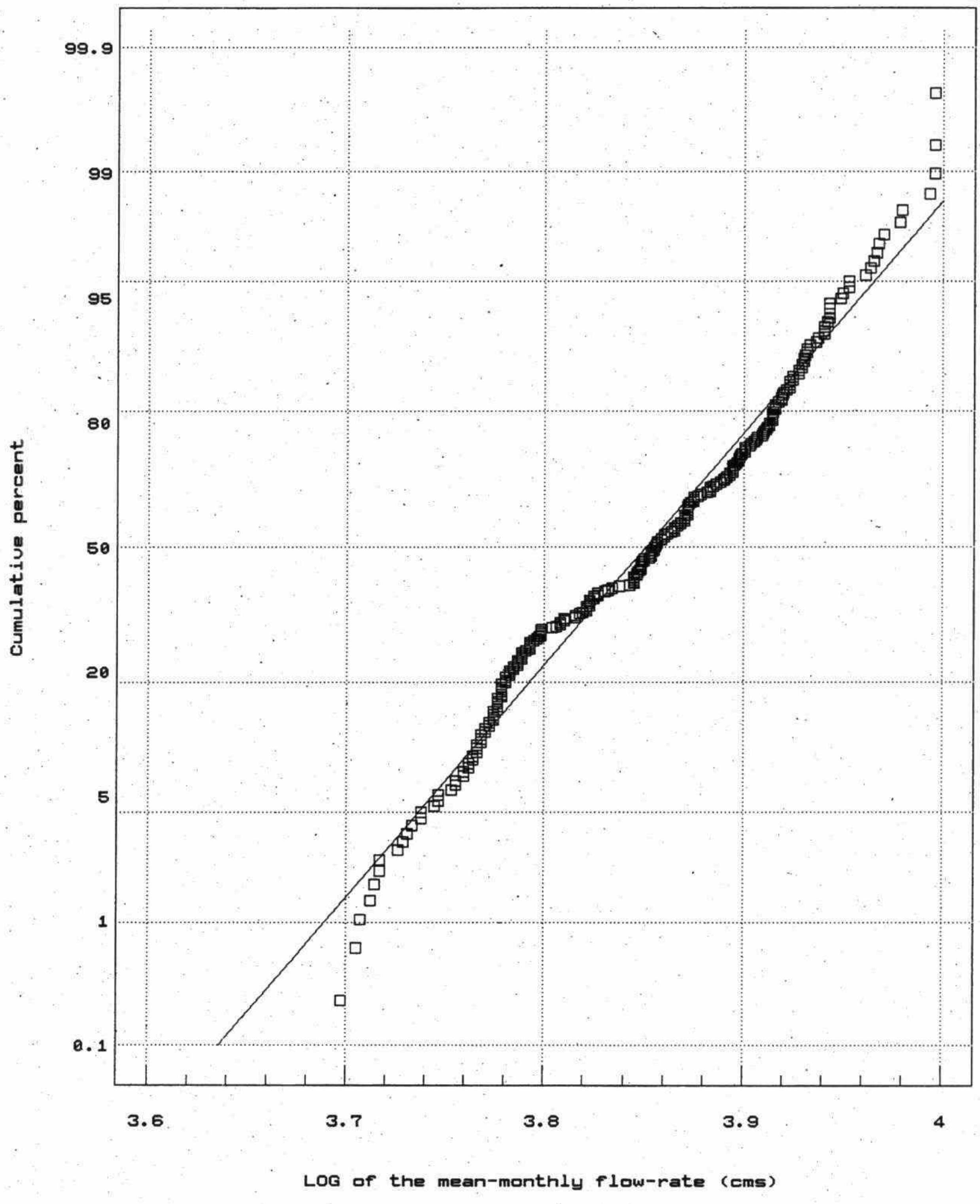


Table 5.1 Basic statistics of lognormal distributions for predicted versus measured model data points and river flow rate.

Parameter		Number of data points	Value of:				
			Mean	Median	Standard Deviation	Minimum	Maximum
I. Ratio of predicted versus measured concentrations (in log units), for:							
a) water column model		16	−0.031	−0.028	0.17	−0.575	0.196
b) sediment model:	Hg	39	−0.0017	0.071	0.827	−2.19	1.50
	Zn	39	0.00009	−0.031	0.309	−0.818	0.80
	PCBs	34	−0.00093	0.131	0.725	−1.86	1.22
c) biota model:	Hg	16	0.0011	−0.011	0.252	−0.568	0.566
	Zn	16	0.0013	−0.047	0.289	−0.486	0.549
	PCBs	8	0.00029	−0.117	0.272	−0.332	0.478
II. Mean−monthly river flow−rate (in log−cms units)		252	3.851	3.855	0.069	3.70	4.00

Figure 5.8 Probability plot of measured mean-monthly river flow-rate.



5.3.2.3 Variability in the river background concentrations:

Based upon limited data [10, 14, 26], it was assumed that the maximum to minimum ratio of river background concentrations (based on the ratio of 97.5 and 2.5 probability percentiles), is 2, for Hg, Zn and PCBs.

5.3.3 Development of the "uncertainty factors", for the parameters

The 5 "uncertainty factors" used in the modified loading limit equations, (Eqs. 5.2 to 5.7, and 4.9), must represent the statistical range of likely values of the corresponding parameter. Further, these data points in the range must be expressed as ratios of the "median" data value, as follows:

$$\textit{uncertainty factor} = \frac{\textit{actual parameter value}}{\textit{median parameter value}} \qquad \ldots\ 5.8$$

Thus for each parameter, the "median uncertainty factor" will have a value of "1", with the other "uncertainty factors" of the range being either less than, or greater than "1". With this definition, the product of a dimensionless "uncertainty factor" and the "median" parameter value, will produce an actual (stochastic) parameter value, (i.e. in correct units).

The minimum number of simulations deemed to be necessary to adequately describe the stochastic nature of the loading limit results, is at most, 250. This number was estimated by using the following: $3^{(\text{parameters})}$ or 3^5. (It should be noted that for the Lake Ontario Monte Carlo analysis, a total of 200 simulations were found sufficient to handle 8 uncertainty parameters which exhibited normal or lognormal distributions, although 300 were used to assure convergence.) A total of 500 "uncertainty factors" were developed for each of the 5 uncertainty parameters, based upon the statistical characteristics of the parameters as described in Section 5.3.2. This was done using the "STATGRAPHICS" (Version 4.0) software package

In order to obtain the dimensionless "uncertainty factors", the actual dimensional data used to assess the statistical distributions described in Section 5.3.2, were divided by the median parameter value. Then, the statistical distribution characteristics describing the resulting dimensionless parameter range, were used to generate 500 parameter values (or "uncertainty factors").

The statistical distribution of the 500 "uncertainty factors" for each parameter are plotted in Figures 5.9 through 5.19. The summary statistics for these "uncertainty factors" are provided in Table 5.2.

Figure 5.9 Probability plot of 500

water column model uncertainty factors.

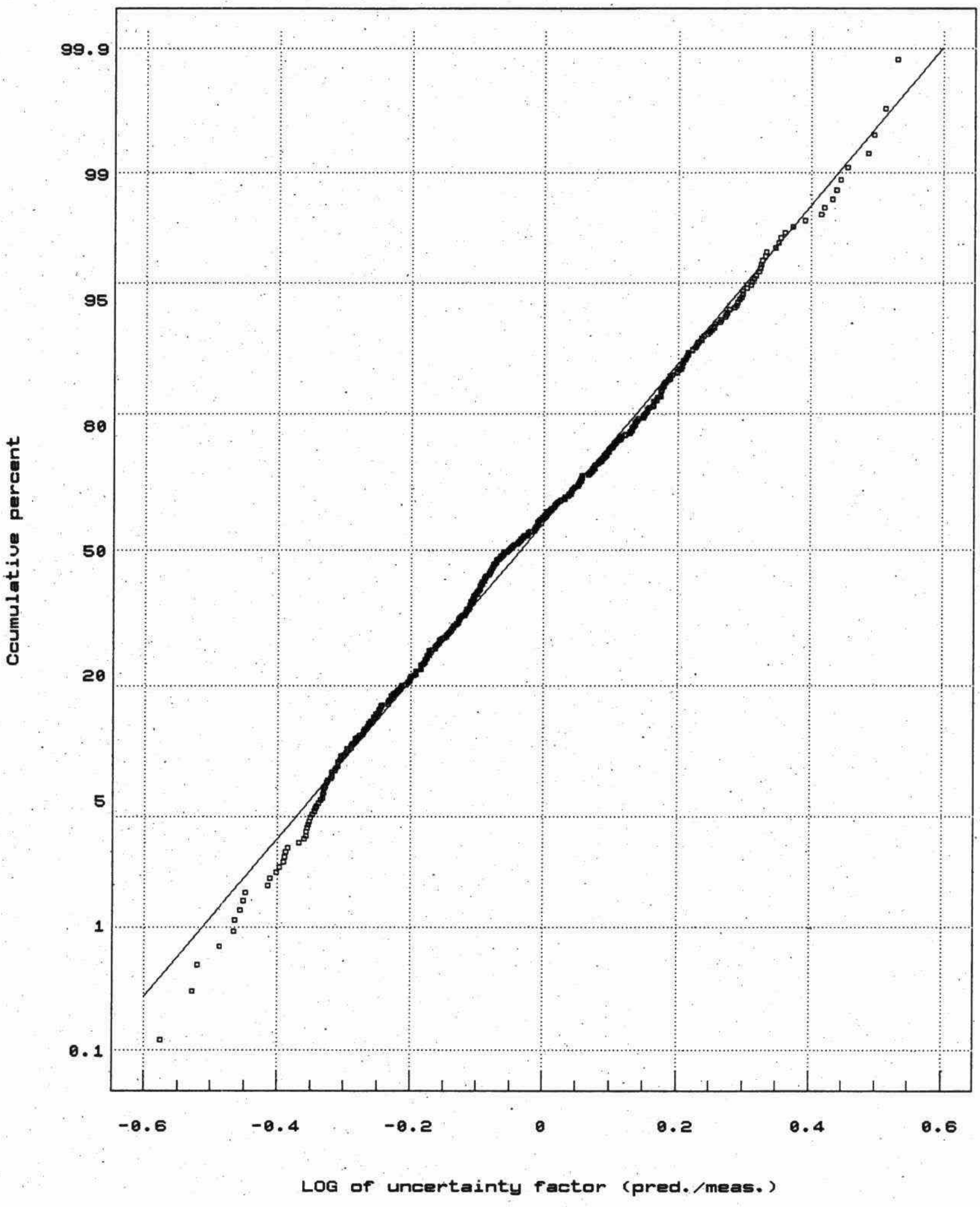


Figure 5.10 Probability plot of 500

Hg sediment model uncertainty factors.

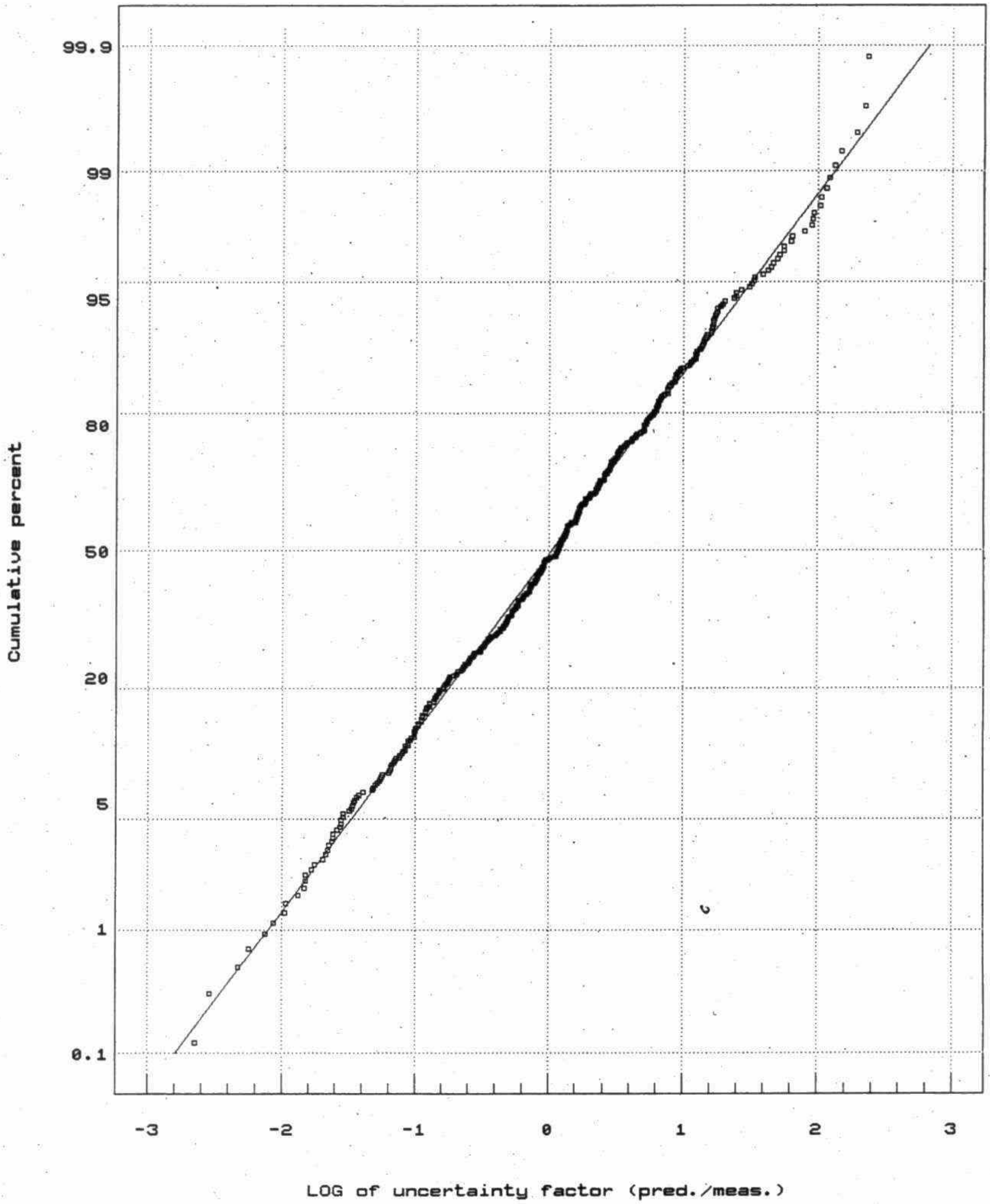


Figure 5.11 Probability plot of 500

Zn sediment model uncertainty factors.

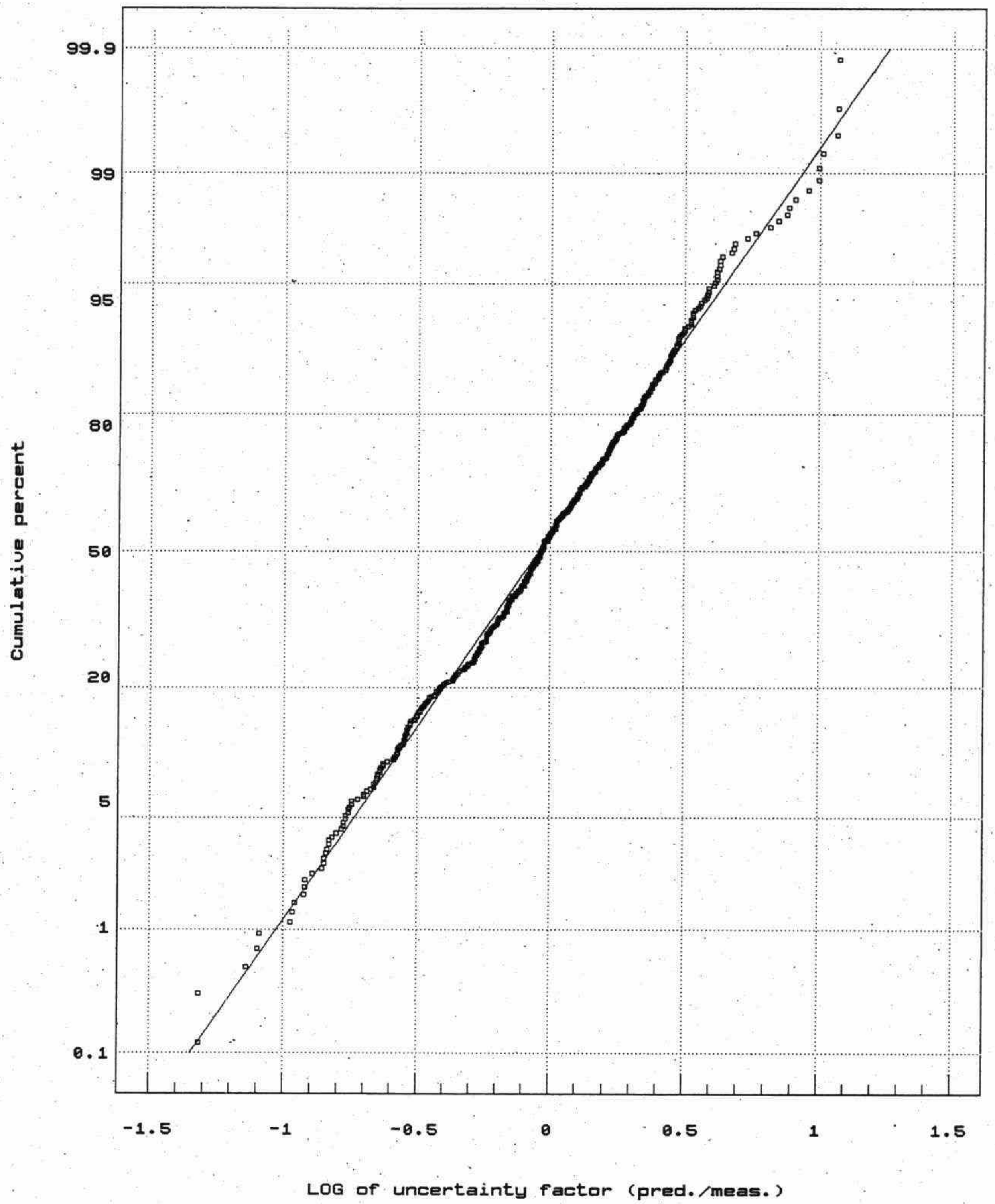


Figure 5.12 Probability plot of 500

PCBs sediment model uncertainty factors.

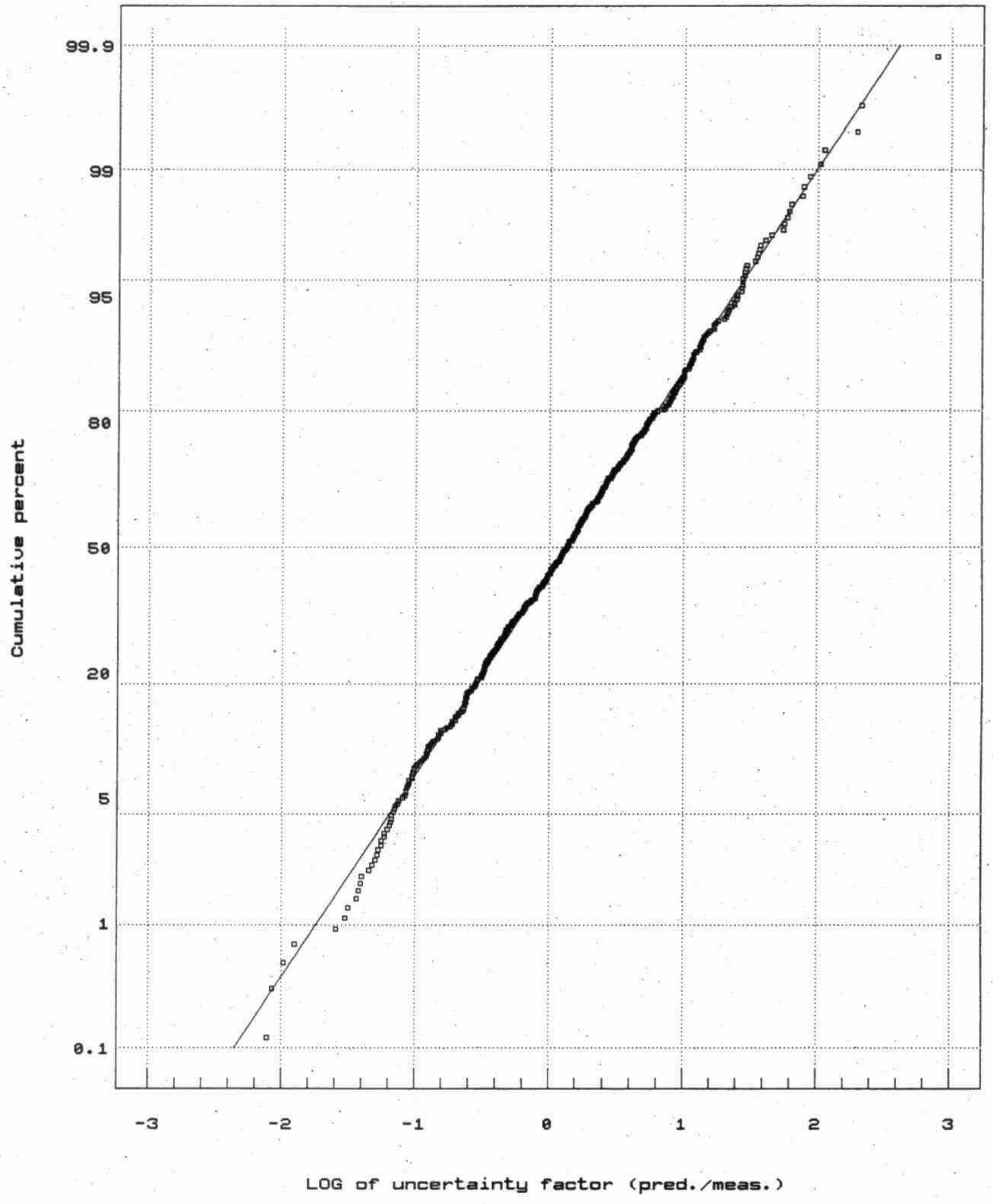


Figure 5.13 Probability plot of 500

m-Hg biota model uncertainty factors.

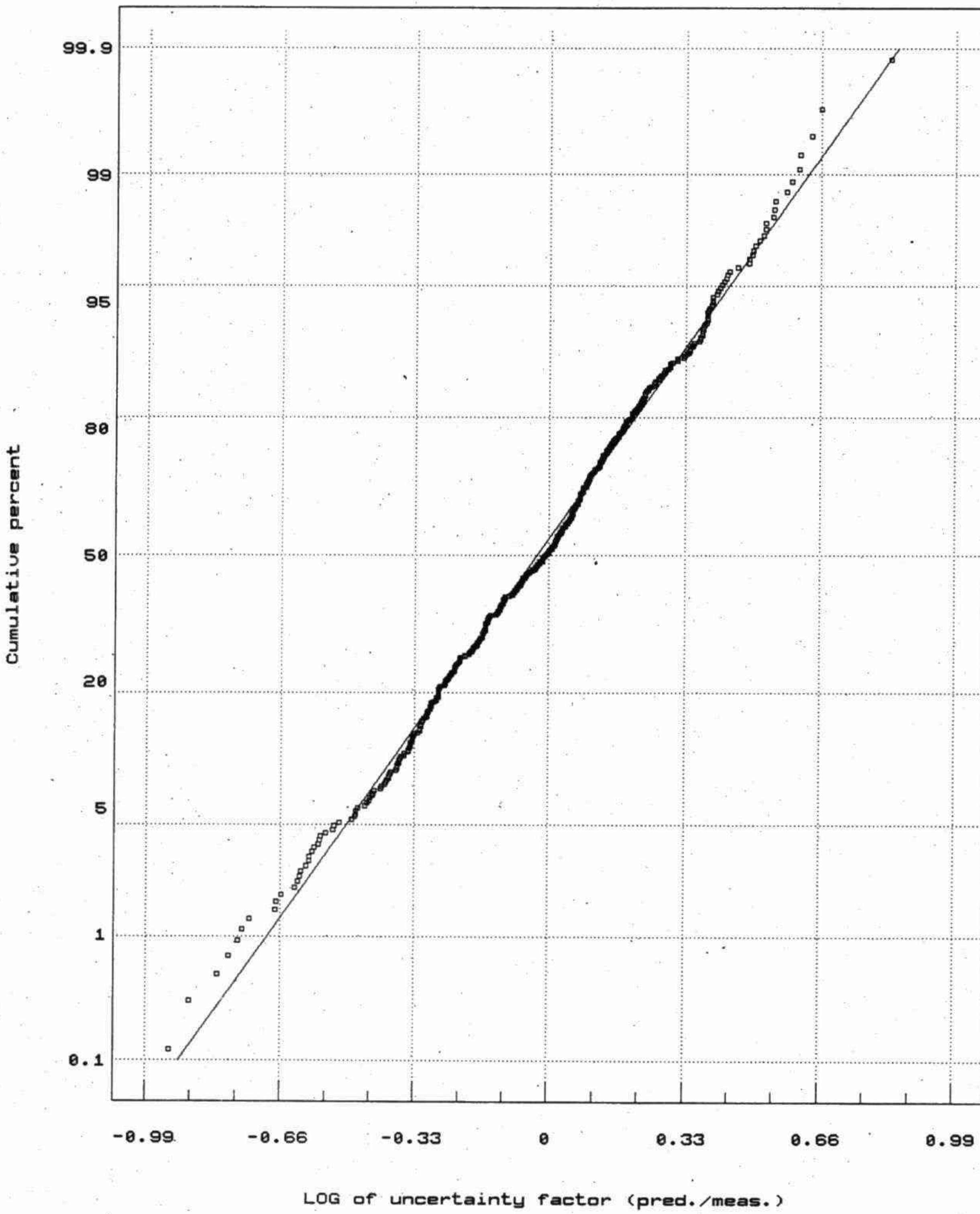


Figure 5.14 Probability plot of 500

Zn biota model uncertainty factors.

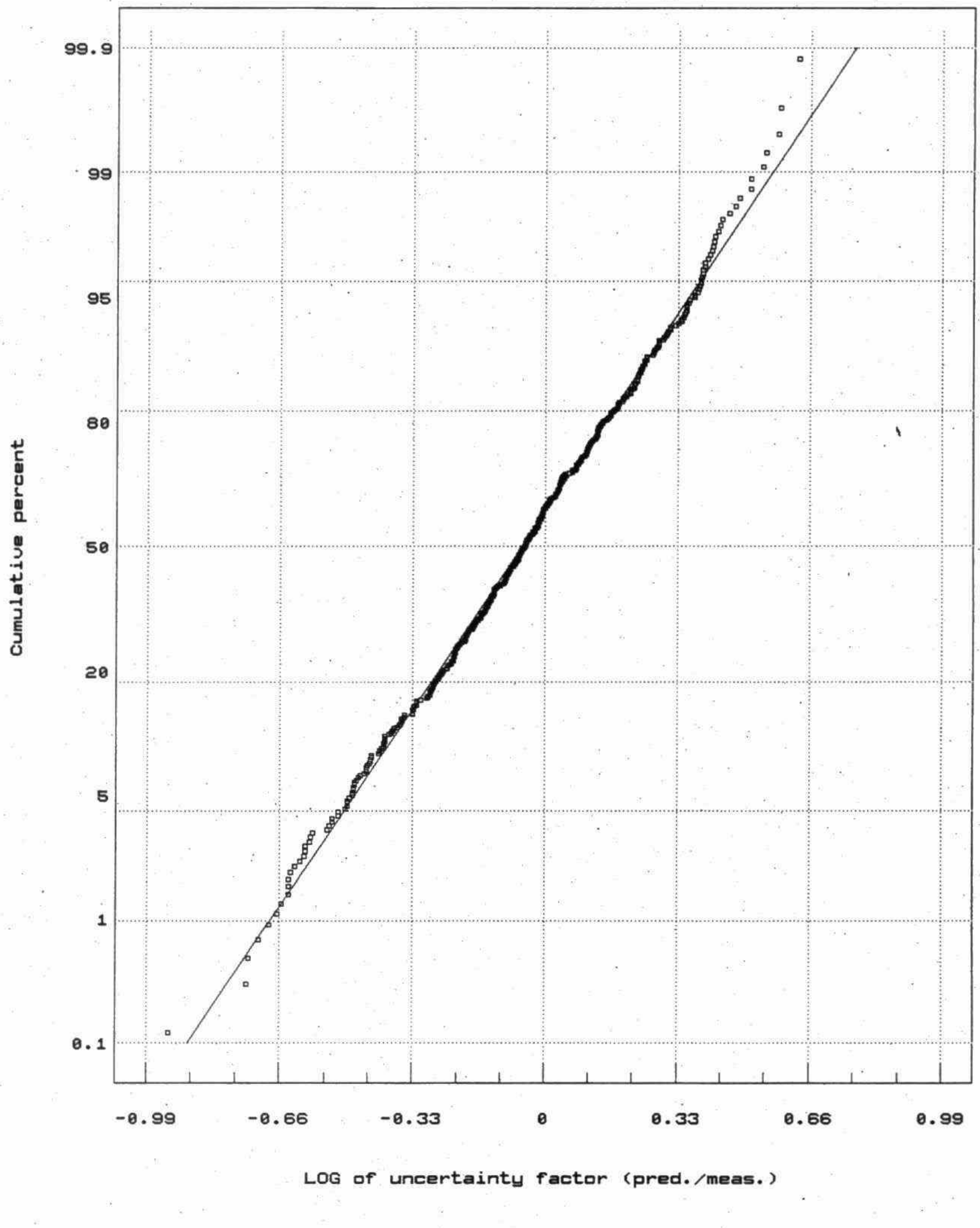


Figure 5.15 Probability plot of 500

PCBs biota model uncertainty factors.

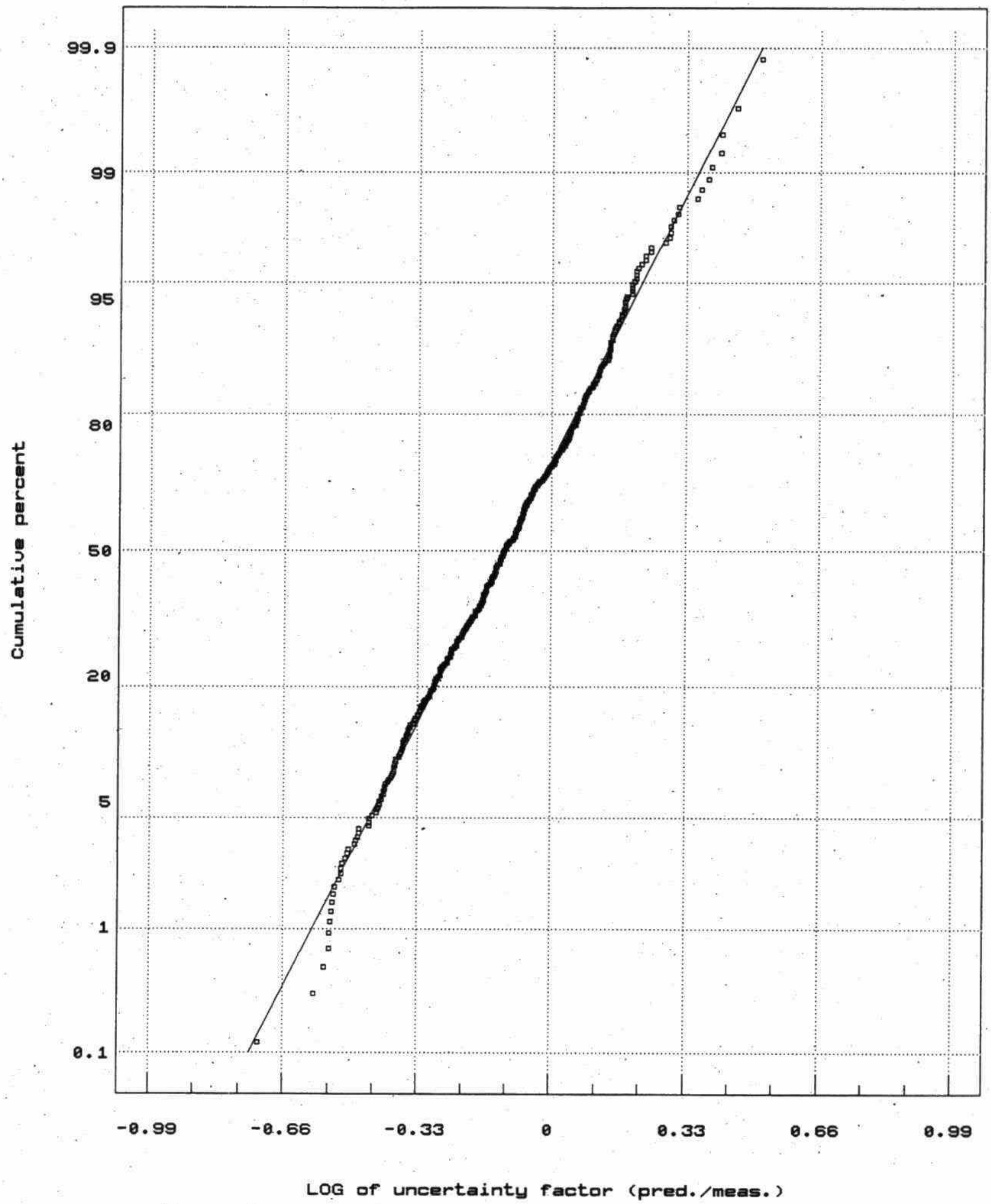


Figure 5.16 Probability plot of 500

Hg background conc. uncertainty factors.

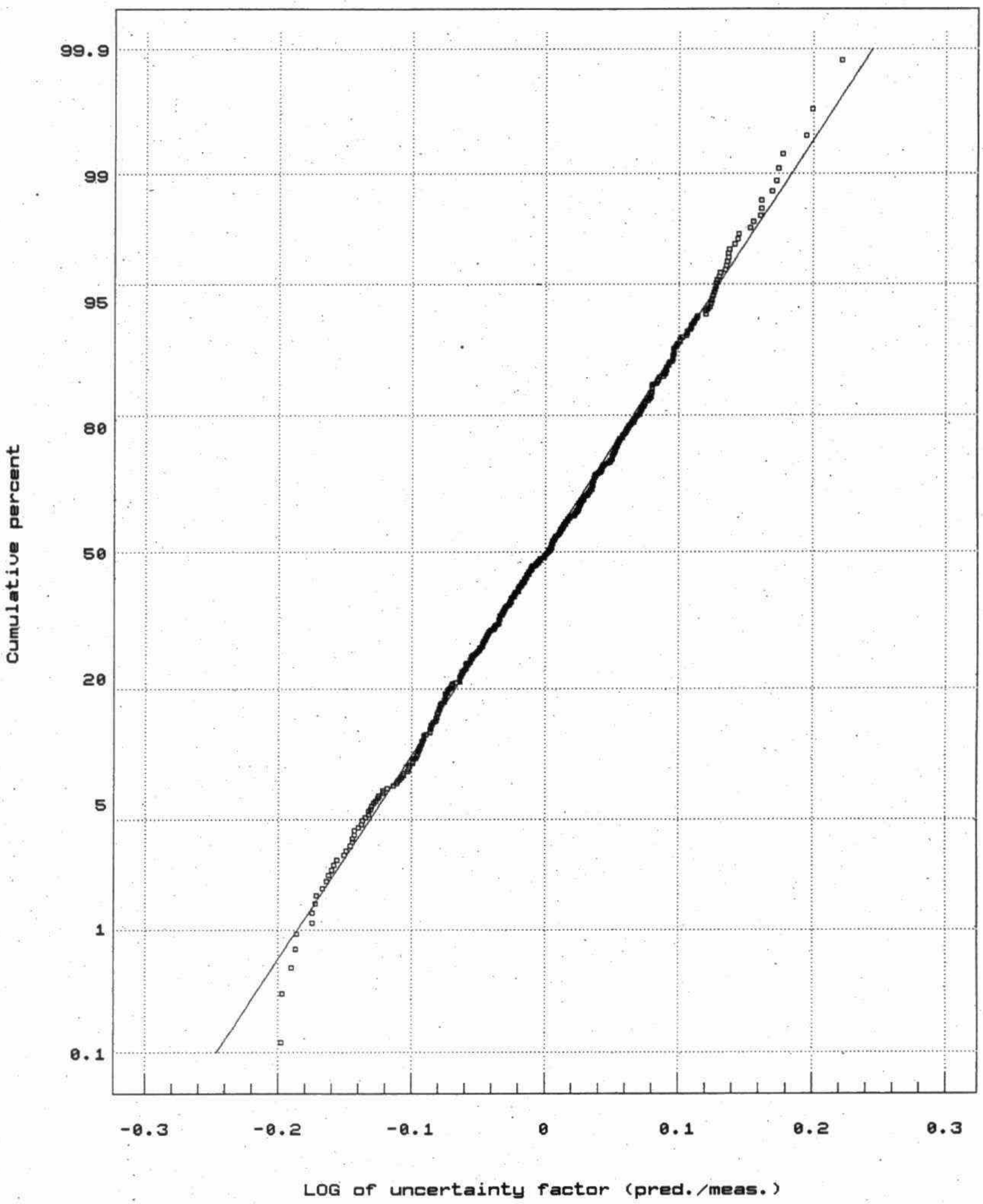


Figure 5.17 Probability plot of 500

Zn background conc. uncertainty factors.

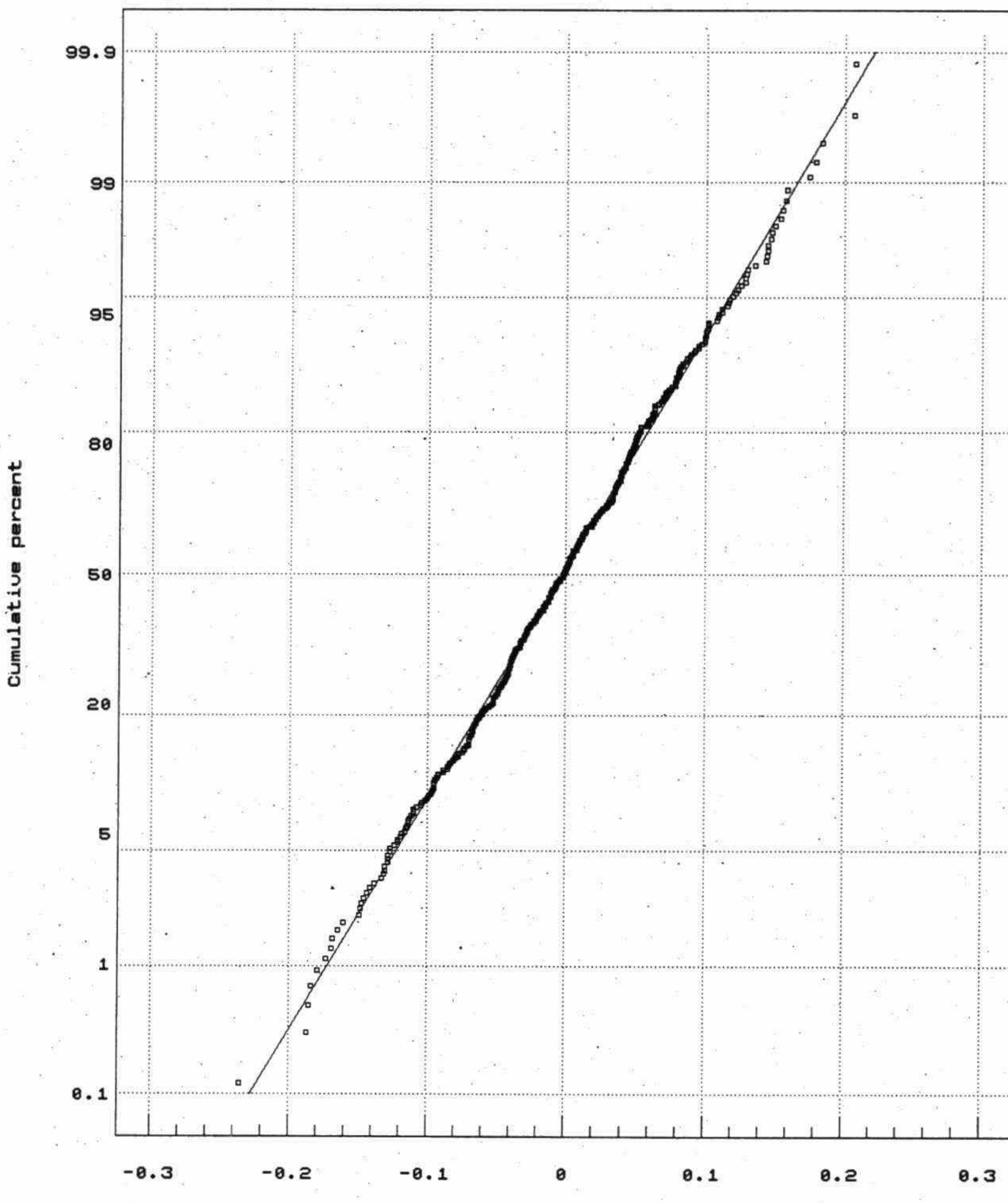


Figure 5.18 Probability plot of 500 PCBs

background conc. uncertainty factors.

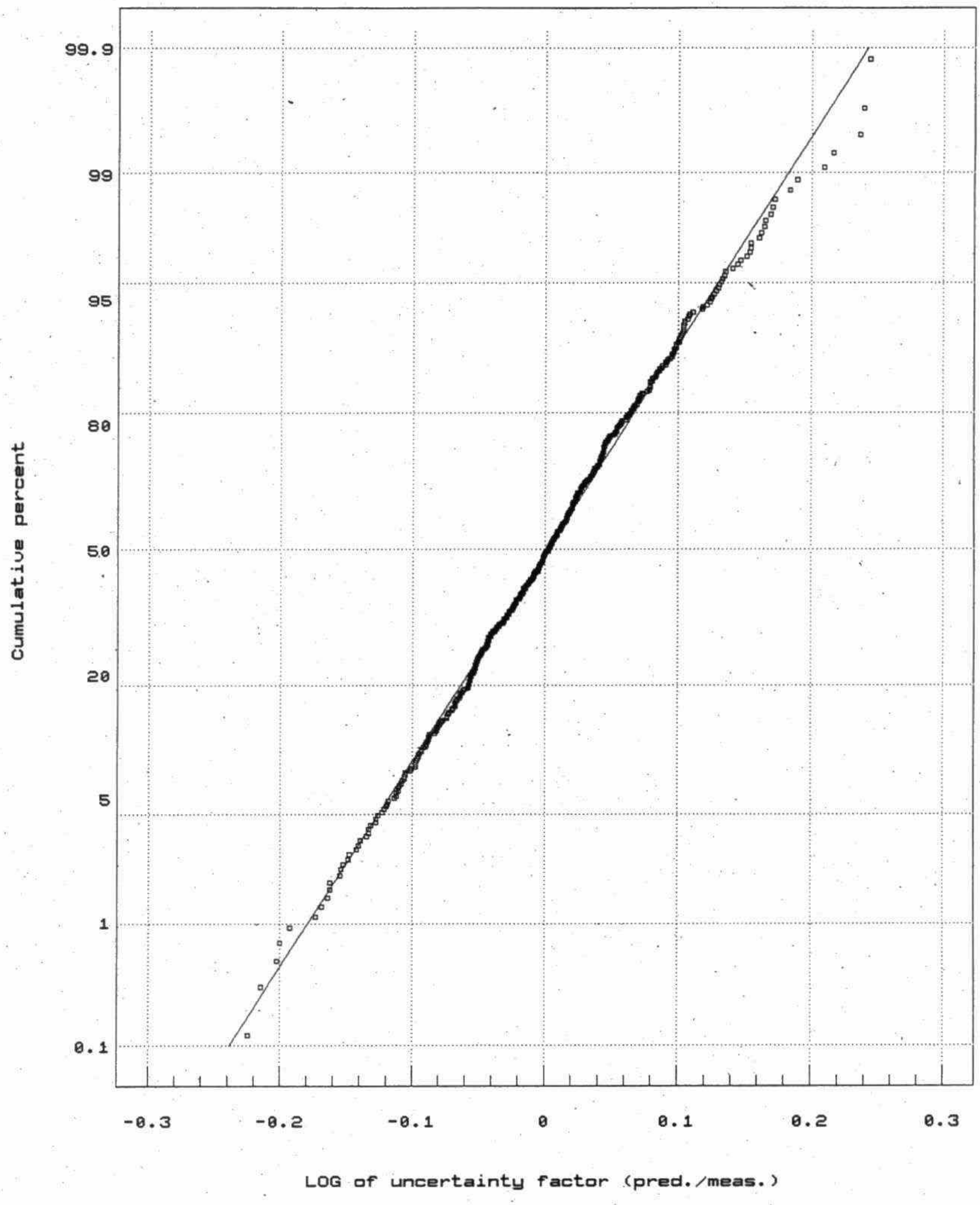


Figure 5.19 Probability plot of 500 river flow-rate uncertainty factors.

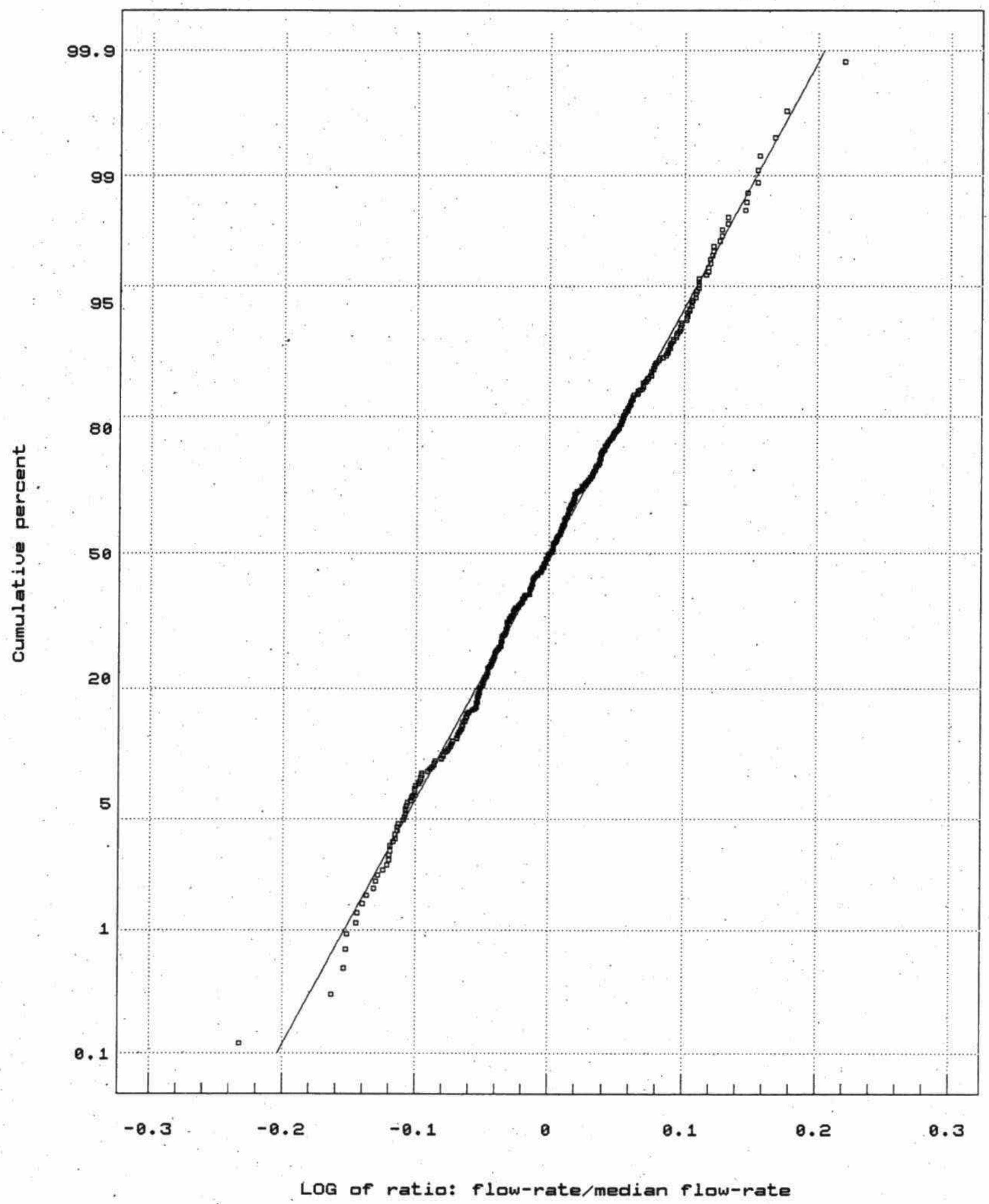


Table 5.2 Basic statistics of the lognormal distributions for the generated uncertainty factors.

Uncertainty parameter:		Number of data points	Value of the "uncertainty factor" of the:				
			Geo. Mean	Median	Standard Deviation	Percentile of: 5 %	Percentile of: 95 %
Water column model accuracy		500	0.923	0.884	0.518	0.447	2.04
Sediment model accuracy for:	Hg	500	1.03	1.15	23.7	0.0285	33.0
	Zn	500	0.903	0.920	1.63	0.170	4.09
	PCBs	500	1.33	1.34	38.9	0.0673	27.7
Biota model accuracy for:	methyl−Hg	500	0.933	0.977	0.788	0.301	2.61
	Zn	500	0.875	0.888	0.663	0.311	2.44
	PCBs	500	0.769	0.763	0.426	0.358	1.58
River flow−rate variability		500	1.00	1.00	0.156	0.778	1.29
River background concentration variability for:	Hg	500	0.999	1.00	0.185	0.731	1.34
	Zn	500	0.993	0.996	0.169	0.747	1.31
	PCBs	500	1.00	1.00	0.186	0.750	1.36

5.4 Results of the "Monte Carlo" simulations

By carrying-out the procedure as outlined, a total of 500 loading limits were obtained for each criterion-chemical-outfall combination. These loading limits were statistically analyzed, (using "STATGRAPHICS"), to obtain the desired "probabilistic loading limits". Since the load allocation parameters are independent of the effluent loading rate, these "probabilistic loading limits" can be used to provide a relationship between the effluent's chemical loading rate and the percentage of the time that the given criterion (upon which, they are derived) would be exceeded.

A total of 3 stochastic applications were made, using the procedure outlined in Section 5.3. These applications examined different components of uncertainty or load allocation strategy. They are used in order to examine the stochastic behaviour of the load allocation model, and to enable recommendations for loading limits to be made. The results are provided in Tables 5.3, 5.4 and 5.5. They are discussed in specific detail later on.

Essentially the tables provide an indication of the percentage of time that the particular criterion would be exceeded under the given constant effluent net loading rate. For example, referring to Table 5.3a: mercury loading rates of about 5.96 and 1.19 kg/day from the Domtar/CIL diffuser, would be expected to exceed the PWQO approximately 95 and 5 % of the time, respectively, (at the ENF of this diffuser).

The negative loading limits in Tables 5.3 and 5.4, occur when the total background concentration (due to both the general river background and local upstream point sources) exceeds the criterion, for the given compliance frequency (percentage of time). Thus from a mathematical perspective, the net loading from the outfall in question would have to be negative in order for the total concentration at the ENF to be lowered to the criterion value. From a practical point of view, negative loading limits should be interpreted as meaning that even with zero net loading, the criterion will be exceeded for the given % of time.

5.4.1 Probabilistic loading limits via load allocation Case IIIb

Probabilistic loading limits based upon meeting the <u>water-column</u> criterion (i.e. "water-based"), were derived using Load allocation Case IIIb for all chemicals. Uncertainty in the value of all key parameters (calibration accuracy, upstream river background concentration and total river flow rate), was considered. For suspended solids only, no background concentration variance was assumed, since the criterion used is directly proportional to the background concentration.

Probabilistic loading limits were also derived based upon meeting the <u>sediment</u> "lowest effect level" (LEL) criterion (i.e. "sediment-based"), for mercury, zinc and total PCBs. They were also derived based upon meeting the chemical body burden criterion in fish (i.e. biota-based), for mercury and total PCBs.

All of the probabilistic loading limits for load allocation Case IIIb are provided in Tables 5.3,

for all outfalls and parameters considered.

The median loading limits provided in Tables 5.3 (i.e. those corresponding to compliance 50 % of the time), are very similar to their corresponding values provided in Tables 4.7, 4.14 and 4.21. The differences, being less than about 30 %, should be considered negligible since the median values of Tables 5.3 were obtained by statistical curve-fitting of the highly variable (log-normal) loading limit functions.

5.4.2 Probabilistic loading limits via load allocation Case IIIb, with ONLY model calibration uncertainty considered

Another application was made in order to examine how the uncertainty associated with the model calibration itself, affects the probabilistic loading limits, (i.e. neglecting the uncertainty introduced by the river flow rate and general river background concentration variabilities). This was accomplished by setting the "RBC" (for all chemicals) and the "RFR" uncertainty factors equal to 1, for all Monte Carlo simulations.

Probabilistic loading limits were derived for mercury, zinc and total PCBs in order to meet both the "Lowest Effect" and "Severe Effect Levels" in sediment. They were also derived for mercury and total PCBs, based upon meeting their respective chemical body burden criterion in the most sensitive aquatic fish species.

The probabilistic loading limits for Case IIIb with model calibration uncertainty only, are provided in Tables 5.4, for mercury, zinc and PCBs.

There is a slight difference between the median values for corresponding loading limits of Tables 5.3 and 5.4. These differences are to be expected, since the results of the two tables were produced via separate curve-fitting exercises.

By comparing the range of loading limits obtained from Tables 5.4, with their corresponding range in Table 5.3, it can be seen that the model calibration accuracy, introduces by far, the largest source of uncertainty into the derived loading limits. For this reason, the loading allocation range is largest for the sediment based limits (since the calibration of the model for this medium, is the least accurate). On the other hand, the load allocation range is smallest for the water-column based limits, (since the calibration of the model for this medium is the most accurate).

The loading limits obtained based upon the water-column criterion for PCBs are all zero since the median general river background concentration is equal to the criterion (1 ng/L), and was assumed for this case not to vary in value. Therefore, the concentration at the ENF would always be equivalent to the criterion, meaning that zero net loadings could be discharged from the outfalls.

5.4.3 Probabilistic loading limits via load allocation Case I

Probabilistic loading limits were also derived based upon load allocation Case I, (i.e. with no background concentrations considered). This was done for mercury, zinc and total PCBs, based upon meeting the respective criterion in the water-column, sediment and aquatic biota.

This was accomplished utilizing the probabilistic loading limit equations for Case IIIb, by simply setting the background concentrations due to impacts from both the general upstream river condition and local upstream point sources, to zero (i.e. $C_{rb} = A_{i,n} = 0$). Uncertainty as caused by model calibration accuracy and river flow rate variability were both considered.

The results for this case are provided in Tables 5.5.

All loading limits obtained using this case are positive in value, since by assumption, there is no background concentrations at all, (and therefore, there would always be some assimilation capacity in the river system for compliance with the criterion in question).

The median loading limits of Tables 5.5 are similar to their corresponding values provided in Tables 4.4, 4.10 and 4.17. The slight difference is due to the curve-fitting of the highly variable (log-normal) load allocation functions for obtaining the values of Tables 5.5.

5.5 Selection of "water quality based loading limits"

The analysis thus far has provided several different loading limits for each parameter from each outfall, depending upon the criterion used, compliance sought, and assumptions made in the uncertainty of the key parameters. Although the analysis serves to illustrate the significance of these factors, it is necessary to select "water quality based loading limits" ("WQBLLs") for recommendation purposes.

In order to derive "WQBLLs", the following steps were used:

1) For each parameter (i.e. Hg, Zn, PCBs, B(a)P, phenols, and suspended solids), the loading limit derived based upon available criteria (i.e. water, sediment - (LEL only), and aquatic biota) are considered.

2) The loading limit used for comparison, is that associated with only 5% exceedence of the respective criterion (i.e. 95% compliance).

3) For the comparison, the following uncertainty assumptions are made:

    a) For meeting the water-column criterion, the limits derived based upon Load Allocation Case IIIb are used (which considers all uncertainty, namely: model calibration, river background concentration and river flow rate). These limits are discussed in Section 5.4.1.

Table 5.3a : **Probabilistic loading limits using Case IIIb – For : MERCURY**

I) Based on criterion for WATER–COLUMN :

% of time exceeded	Loading (kg/day), for outfall:				
	Dom/CIL	Court–VS	Court–A	Court–S	WPCP
99	7.8535	3.5725	3.252	0.0871	1.054
97.5	6.843	3.113	2.834	0.07589	0.9184
95	5.964	2.713	2.47	0.066145	0.80045
90	5.406	2.459	2.2385	0.059955	0.72555
80	4.17	1.897	1.727	0.04625	0.5597
75	3.819	1.7375	1.5815	0.042355	0.51255
50	2.7715	1.261	1.1475	0.03074	0.372
25	1.912	0.86975	0.7918	0.021205	0.25665
20	1.7595	0.8004	0.72865	0.019515	0.23615
10	1.427	0.6491	0.59095	0.01583	0.1915
5	1.1875	0.54015	0.4917	0.01317	0.15935
2.5	1.031	0.4692	0.4271	0.01144	0.1384
1	0.8461	0.3849	0.3504	0.009384	0.1136

II) Based on criterion for SEDIMENT (LEL) :

% of time exceeded	Loading (kg/day), for outfall:				
	Dom/CIL	Court–VS	Court–A	Court–S	WPCP
99	46.275	21.05	19.165	0.51325	6.211
97.5	25.08	11.41	10.39	0.2782	3.366
95	12.515	5.693	5.1825	0.1388	1.6795
90	5.3815	2.448	2.229	0.05969	0.7223
80	2.109	0.9593	0.87335	0.02339	0.28305
75	1.4285	0.64985	0.5916	0.015845	0.19175
50	0.30775	0.13995	0.12745	0.003413	0.041305
25	−0.02513	−0.01143	−0.0104	−0.00028	−0.00337
20	−0.06682	−0.0304	−0.02768	−0.00074	−0.00897
10	−0.10665	−0.04853	−0.04418	−0.00118	−0.01432
5	−0.13515	−0.06147	−0.05596	−0.0015	−0.01814
2.5	−0.1515	−0.06892	−0.06274	−0.00168	−0.02033
1	−0.1646	−0.0749	−0.06819	−0.00183	−0.0221

III) Based on criterion for BIOTA (body burden) :

% of time exceeded	Loading (kg/day), for outfall:				
	Dom/CIL	Court–VS	Court–A	Court–S	WPCP
99	17.59	8.001	7.284	0.1951	2.361
97.5	15.96	7.262	6.611	0.1771	2.143
95	13.41	6.0985	5.552	0.1487	1.799
90	10.475	4.764	4.337	0.11615	1.4055
80	7.6195	3.4665	3.1555	0.08451	1.023
75	6.701	3.0485	2.7755	0.074325	0.89935
50	4.443	2.0215	1.84	0.049275	0.5963
25	2.7695	1.26	1.147	0.03072	0.37175
20	2.526	1.149	1.046	0.028015	0.33905
10	1.8505	0.8418	0.76635	0.02052	0.24835
5	1.375	0.6254	0.5694	0.01525	0.18455
2.5	1.009	0.4591	0.418	0.01119	0.1355
1	0.61925	0.2817	0.25645	0.006868	0.083115

Table 5.3b : Probabilistic loading limits using Case IIIb – For : ZINC

I) Based on criterion for WATER–COLUMN :

% of time exceeded	Loading (kg/day), for outfall:				
	Dom/CIL	Court–VS	Court–A	Court–S	WPCP
99	1178.5	536.05	488	13.07	158.15
97.5	1008	458.7	417.6	11.18	135.3
95	887.15	403.55	367.4	9.839	119.1
90	793.8	361.1	328.7	8.804	106.5
80	617.8	281.05	255.85	6.8515	82.915
75	558.4	254	231.25	6.1935	74.95
50	411.5	187.15	170.45	4.564	55.225
25	281.85	128.25	116.75	3.126	37.83
20	258.45	117.55	107.05	2.866	34.685
10	212.75	96.76	88.09	2.3595	28.55
5	174.85	79.55	72.42	1.9395	23.47
2.5	151.9	69.1	62.9	1.685	20.39
1	126.35	57.48	52.33	1.4015	16.96

II) Based on criterion for SEDIMENT (LEL) :

% of time exceeded	Loading (kg/day), for outfall:				
	Dom/CIL	Court–VS	Court–A	Court–S	WPCP
99	768.25	349.45	318.15	8.5205	103.13
97.5	436.2	198.4	180.6	4.838	58.55
95	279.1	127	115.6	3.0955	37.46
90	199.1	90.575	82.465	2.2085	26.725
80	133.4	60.685	55.245	1.4795	17.905
75	108.65	49.425	44.995	1.205	14.585
50	44.145	20.08	18.28	0.4896	5.9255
25	12.38	5.6315	5.127	0.1373	1.6615
20	4.344	1.9765	1.799	0.04818	0.58305
10	−7.7225	−3.5125	−3.198	−0.08565	−1.0365
5	−15.29	−6.956	−6.3325	−0.1696	−2.052
2.5	−16.77	−7.627	−6.943	−0.186	−2.25
1	−20.655	−9.3935	−8.552	−0.22905	−2.7715

III) Based on criterion for BIOTA (body burden) :

% of time exceeded	Loading (kg/day), for outfall:				
	Dom/CIL	Court–VS	Court–A	Court–S	WPCP
99					
97.5					
95					
90					
80					
75					
50					
25					
20					
10					
5					
2.5					
1					

Table 5.3c : Probabilistic loading limits using Case IIIb – For : total PCBs

I) Based on criterion for WATER–COLUMN :

% of time	Loading (kg/day), for outfall:				
exceeded	Dom/CIL	Court–VS	Court–A	Court–S	WPCP
99	0.007004	0.003186	0.0029	0.000078	0.00094
97.5	0.00525	0.002388	0.002174	0.000058	0.000705
95	0.004021	0.001829	0.001666	0.000045	0.00054
90	0.002972	0.001352	0.001231	0.000033	0.000399
80	0.001751	0.000797	0.000725	0.000019	0.000235
75	0.001411	0.000642	0.000584	0.000016	0.000189
50	−5.6E−05	−2.5E−05	−2.3E−05	−6.2E−07	−7.5E−06
25	−0.00181	−0.00083	−0.00075	−2.0E−05	−0.00024
20	−0.00243	−0.00111	−0.00101	−2.7E−05	−0.00033
10	−0.00396	−0.0018	−0.00164	−4.4E−05	−0.00053
5	−0.00621	−0.00282	−0.00257	−6.9E−05	−0.00083
2.5	−0.00731	−0.00333	−0.00303	−8.1E−05	−0.00098
1	−0.00894	−0.00406	−0.0037	−9.9E−05	−0.0012

II) Based on criterion for SEDIMENT (LEL) :

% of time	Loading (kg/day), for outfall:				
exceeded	Dom/CIL	Court–VS	Court–A	Court–S	WPCP
99	1.0305	0.4688	0.4268	0.01143	0.13835
97.5	0.5212	0.2371	0.2159	0.005781	0.06996
95	0.29565	0.1345	0.12245	0.003279	0.03968
90	0.1511	0.06873	0.06257	0.001676	0.020275
80	0.06248	0.02842	0.025875	0.000693	0.008386
75	0.03853	0.017525	0.01596	0.000427	0.005172
50	0.002071	0.000942	0.000857	0.000023	0.000278
25	−0.00877	−0.00399	−0.00363	−9.7E−05	−0.00118
20	−0.01032	−0.00469	−0.00427	−0.00011	−0.00138
10	−0.01289	−0.00586	−0.00534	−0.00014	−0.00173
5	−0.01499	−0.00682	−0.00621	−0.00017	−0.00201
2.5	−0.01626	−0.0074	−0.00674	−0.00018	−0.00218
1	−0.01863	−0.00848	−0.00772	−0.00021	−0.0025

III) Based on criterion for BIOTA (body burden) :

% of time	Loading (kg/day), for outfall:				
exceeded	Dom/CIL	Court–VS	Court–A	Court–S	WPCP
99	−0.00268	−0.00122	−0.00111	−3.0E−05	−0.00036
97.5	−0.00451	−0.00205	−0.00187	−5.0E−05	−0.0006
95	−0.00533	−0.00242	−0.00221	−5.9E−05	−0.00072
90	−0.00635	−0.00289	−0.00263	−7.0E−05	−0.00085
80	−0.00741	−0.00337	−0.00307	−8.2E−05	−0.00099
75	−0.00791	−0.0036	−0.00328	−8.8E−05	−0.00106
50	−0.01008	−0.00459	−0.00417	−0.00011	−0.00135
25	−0.01242	−0.00565	−0.00514	−0.00014	−0.00167
20	−0.01301	−0.00592	−0.00539	−0.00014	−0.00175
10	−0.01468	−0.00668	−0.00608	−0.00016	−0.00197
5	−0.01606	−0.0073	−0.00665	−0.00018	−0.00215
2.5	−0.01789	−0.00814	−0.00741	−0.0002	−0.0024
1	−0.01944	−0.00884	−0.00805	−0.00022	−0.00261

Table 5.3d : Probabilistic loading limits using Case IIIb – For : B(a)P

Based on criterion for WATER–COLUMN :

% of time exceeded	Loading (grams/day), for outfall:				
	Dom/CIL	Court–VS	Court–A	Court–S	WPCP
99	2.5245	1.1485	1.0455	0.028	0.33885
97.5	2.174	0.989	0.9003	0.02411	0.2918
95	1.899	0.86385	0.7864	0.021065	0.25485
90	1.7045	0.77525	0.70575	0.018905	0.22875
80	1.318	0.5995	0.54575	0.014615	0.17685
75	1.1975	0.5447	0.4959	0.01328	0.1607
50	0.87685	0.39885	0.3631	0.009725	0.11765
25	0.60645	0.27585	0.25115	0.006727	0.081395
20	0.55235	0.2513	0.22875	0.006126	0.074135
10	0.4543	0.20665	0.18815	0.005039	0.06098
5	0.37485	0.1705	0.1552	0.004157	0.05031
2.5	0.3268	0.1487	0.1353	0.003625	0.04386
1	0.26905	0.1224	0.1114	0.002984	0.036115

Table 5.3e : Probabilistic loading limits using Case IIIb – For : Phenols

Based on criterion for WATER–COLUMN :

% of time exceeded	Loading (kg/day), for outfall:				
	Dom/CIL	Court–VS	Court–A	Court–S	WPCP
99	42.015	19.11	17.4	0.46595	5.639
97.5	36.18	16.46	14.98	0.4013	4.856
95	31.615	14.38	13.09	0.3506	4.2425
90	28.375	12.91	11.75	0.3147	3.808
80	21.94	9.9815	9.085	0.2433	2.9445
75	19.935	9.0685	8.256	0.2211	2.6755
50	14.6	6.642	6.0465	0.16195	1.9595
25	10.095	4.593	4.1815	0.112	1.355
20	9.1965	4.1835	3.8085	0.102	1.234
10	7.563	3.44	3.132	0.08388	1.015
5	6.2405	2.8385	2.5845	0.069215	0.83755
2.5	5.44	2,475	2.253	0.06034	0.7302
1	4.479	2.037	1.8545	0.049675	0.6011

Table 5.3f : Probabilistic loading limits using Case IIIb – For : Sus. solids

Based on criterion for WATER–COLUMN :

% of time exceeded	Loading (kg/day), for outfall:				
	Dom/CIL	Court–VS	Court–A	Court–S	WPCP
99	3787	1722.5	1568	42	508.25
97.5	3261	1483	1351	36.17	437.7
95	2848.5	1296	1179.5	31.59	382.35
90	2556.5	1163	1058.5	28.35	343.15
80	1976.5	899.2	818.65	21.925	265.3
75	1796.5	817.1	743.85	19.92	241.05
50	1315.5	598.3	544.7	14.59	176.5
25	909.7	413.8	376.7	10.09	122.1
20	828.55	376.9	343.1	9.1895	111.2
10	681.5	310.05	282.2	7.5585	91.465
5	562.3	255.8	232.85	6.2365	75.465
2.5	490.2	223	203	5.437	65.79
1	403.55	183.6	167.15	4.476	54.17

Table 5.4a: Probabilistic loading limits using Case IIIb, with only model calibration uncertainty considered – For : MERCURY

I) Based on criterion for WATER–COLUMN :

% of time exceeded	Loading (kg/day), for outfall:				
	Dom/CIL	Court–VS	Court–A	Court–S	WPCP
99	7.3145	3.3275	3.029	0.081125	0.9817
97.5	6.261	2.848	2.593	0.06944	0.8403
95	5.6235	2.558	2.329	0.06237	0.75475
90	5.0655	2.3045	2.0975	0.056175	0.6798
80	4.1145	1.872	1.704	0.045635	0.5522
75	3.7785	1.7185	1.565	0.041905	0.5071
50	2.8425	1.2935	1.177	0.031525	0.3815
25	1.9515	0.8877	0.80815	0.021645	0.2619
20	1.7755	0.8076	0.7352	0.01969	0.2383
10	1.4765	0.67165	0.61145	0.016375	0.1982
5	1.2295	0.5594	0.5093	0.01364	0.16505
2.5	1.094	0.4977	0.4531	0.01213	0.1468
1	0.88995	0.40485	0.36855	0.00987	0.1194

II) Based on criterion for SEDIMENT (LEL) :

% of time exceeded	Loading (kg/day), for outfall:				
	Dom/CIL	Court–VS	Court–A	Court–S	WPCP
99	48.5	22.06	20.09	0.53795	6.51
97.5	30.41	13.83	12.59	0.3373	4.081
95	12.525	5.6965	5.186	0.13885	1.6805
90	5.391	2.4525	2.2325	0.05979	0.7235
80	2.2015	1.0015	0.91175	0.024415	0.2955
75	1.453	0.66095	0.60175	0.016115	0.19505
50	0.30805	0.1401	0.12755	0.003416	0.04134
25	−0.03477	−0.01582	−0.0144	−0.00039	−0.00467
20	−0.06984	−0.03177	−0.02893	−0.00077	−0.00937
10	−0.10515	−0.04784	−0.04355	−0.00117	−0.01412
5	−0.1213	−0.05518	−0.05024	−0.00135	−0.01629
2.5	−0.1258	−0.05724	−0.05211	−0.0014	−0.01689
1	−0.12915	−0.05875	−0.05348	−0.00143	−0.01733

III) Based on criterion for SEDIMENT (SEL) :

% of time exceeded	Loading (kg/day), for outfall:				
	Dom/CIL	Court–VS	Court–A	Court–S	WPCP
99	479.5	218.15	198.55	5.3185	64.36
97.5	301.1	137	124.7	3.339	40.41
95	124.7	56.71	51.625	1.383	16.73
90	54.34	24.715	22.505	0.60265	7.293
80	22.885	10.41	9.4765	0.2538	3.071
75	15.505	7.0515	6.4195	0.1719	2.0805
50	4.21	1.915	1.7435	0.04669	0.565
25	0.82905	0.3771	0.34335	0.009195	0.1113
20	0.4831	0.21975	0.2001	0.005358	0.064845
10	0.1347	0.061285	0.055795	0.001495	0.01808
5	−0.02437	−0.01109	−0.01009	−0.00027	−0.00327
2.5	−0.06911	−0.03144	−0.02862	−0.00077	−0.00928
1	−0.10168	−0.04625	−0.0421	−0.00113	−0.01365

IV) Based on criterion for BIOTA (body burden) :

% of time exceeded	Loading (kg/day), for outfall:				
	Dom/CIL	Court–VS	Court–A	Court–S	WPCP
99	18.87	8.584	7.8145	0.2093	2.5325
97.5	15.72	7.15	6.51	0.1743	2.11
95	12.365	5.624	5.1205	0.13715	1.6595
90	10.515	4.7825	4.354	0.1166	1.411
80	7.4545	3.391	3.087	0.082675	1.00065
75	6.656	3.028	2.7565	0.073825	0.8934
50	4.5465	2.0685	1.883	0.05043	0.6102
25	2.703	1.2295	1.1195	0.029975	0.36275
20	2.428	1.1045	1.0055	0.02693	0.32595
10	1.901	0.8648	0.78735	0.021085	0.25515
5	1.307	0.59445	0.5412	0.014495	0.1754
2.5	1.035	0.4706	0.4284	0.01147	0.1388
1	0.7007	0.31875	0.29015	0.007772	0.094045

Table 5.4b: Probabilistic loading limits using Case IIIb, with only model calibration uncertainty considered – For : ZINC

I) Based on criterion for WATER–COLUMN :

% of time exceeded	Loading (kg/day), for outfall:				
	Dom/CIL	Court–VS	Court–A	Court–S	WPCP
99	1078	490.3	446.4	11.955	144.7
97.5	922.7	419.7	382.1	10.23	123.8
95	828.7	377	343.2	9.191	111.2
90	746.5	339.6	309.1	8.279	100.2
80	606.35	275.85	251.1	6.725	81.38
75	556.8	253.3	230.6	6.1755	74.73
50	418.9	190.55	173.45	4.6465	56.22
25	287.6	130.8	119.1	3.1895	38.6
20	261.65	119.05	108.35	2.9015	35.115
10	217.6	98.98	90.115	2.4135	29.205
5	181.2	82.44	75.05	2.01	24.325
2.5	161.2	73.34	66.77	1.788	21.64
1	131.15	59.66	54.31	1.4545	17.6

II) Based on criterion for SEDIMENT (LEL) :

% of time exceeded	Loading (kg/day), for outfall:				
	Dom/CIL	Court–VS	Court–A	Court–S	WPCP
99	736.6	335.05	305.05	8.1695	98.86
97.5	418.1	190.2	173.1	4.637	56.11
95	288.45	131.2	119.45	3.1985	38.71
90	204.1	92.85	84.53	2.264	27.395
80	131.7	59.895	54.53	1.46	17.675
75	107.1	48.72	44.355	1.188	14.375
50	44.48	20.23	18.42	0.4933	5.97
25	13.34	6.0675	5.524	0.14795	1.7905
20	3.232	1.4705	1.3385	0.03585	0.4338
10	−6.4995	−2.9565	−2.6915	−0.07209	−0.87235
5	−13.375	−6.085	−5.5395	−0.14835	−1.7955
2.5	−15.74	−7.159	−6.517	−0.1745	−2.112
1	−19.21	−8.736	−7.9535	−0.213	−2.5775

III) Based on criterion for SEDIMENT (SEL) :

% of time exceeded	Loading (kg/day), for outfall:				
	Dom/CIL	Court–VS	Court–A	Court–S	WPCP
99	5188	2360	2148.5	57.535	696.25
97.5	3011	1370	1247	33.4	404.2
95	2125	966.75	880.1	23.57	285.25
90	1549.5	704.7	641.55	17.185	207.9
80	1054	479.45	436.5	11.69	141.5
75	886.2	403.15	367	9.829	118.9
50	458.25	208.45	189.75	5.0825	61.5
25	245.45	111.65	101.65	2.722	32.94
20	176.4	80.23	73.04	1.956	23.675
10	109.85	49.98	45.5	1.2185	14.745
5	62.87	28.6	26.035	0.6973	8.438
2.5	46.75	21.26	19.36	0.5185	6.274
1	23.045	10.485	9.5425	0.2556	3.093

IV) Based on criterion for BIOTA (body burden) :

% of time exceeded	Loading (kg/day), for outfall:				
	Dom/CIL	Court–VS	Court–A	Court–S	WPCP
99					
97.5					
95					
90					
80					
75					
50					
25					
20					
10					
5					
2.5					
1					

Table 5.4c : Probabilistic loading limits using Case IIIb, with only model calibration uncertainty considered – For : PCBs

I) Based on criterion for WATER–COLUMN :

% of time	Loading (kg/day), for outfall:				
exceeded	Dom/CIL	Court–VS	Court–A	Court–S	WPCP
99	0	0	0	0	0
97.5	0	0	0	0	0
95	0	0	0	0	0
90	0	0	0	0	0
80	0	0	0	0	0
75	0	0	0	0	0
50	0	0	0	0	0
25	0	0	0	0	0
20	0	0	0	0	0
10	0	0	0	0	0
5	0	0	0	0	0
2.5	0	0	0	0	0
1	0	0	0	0	0

II) Based on criterion for SEDIMENT (LEL) :

% of time	Loading (kg/day), for outfall:				
exceeded	Dom/CIL	Court–VS	Court–A	Court–S	WPCP
99	1.0717	0.4875	0.44375	0.011885	0.14385
97.5	0.614	0.2793	0.2543	0.00681	0.0824
95	0.3002	0.13655	0.12435	0.00333	0.040295
90	0.14395	0.06549	0.05962	0.001597	0.01932
80	0.058655	0.026685	0.02429	0.000651	0.007873
75	0.036455	0.01658	0.015095	0.000404	0.004893
50	0.001895	0.000862	0.000785	0.000021	0.000254
25	−0.00919	−0.00418	−0.0038	−0.0001	−0.00123
20	−0.01006	−0.00458	−0.00417	−0.00011	−0.00135
10	−0.01186	−0.0054	−0.00491	−0.00013	−0.00159
5	−0.01247	−0.00567	−0.00516	−0.00014	−0.00167
2.5	−0.01269	−0.00577	−0.00526	−0.00014	−0.0017
1	−0.01291	−0.00587	−0.00535	−0.00014	−0.00173

III) Based on criterion for SEDIMENT (SEL) :

% of time	Loading (kg/day), for outfall:				
exceeded	Dom/CIL	Court–VS	Court–A	Court–S	WPCP
99	288	131.05	119.3	3.1945	38.655
97.5	166.5	75.74	68.95	1.847	22.35
95	83.2	37.85	34.455	0.92275	11.165
90	41.72	18.98	17.28	0.46275	5.5995
80	19.07	8.6745	7.8975	0.2115	2.5595
75	13.18	5.9935	5.456	0.1461	1.7685
50	4.001	1.8195	1.657	0.044375	0.53695
25	1.059	0.4818	0.43865	0.011745	0.14215
20	0.8269	0.37615	0.34245	0.009171	0.11095
10	0.348	0.1583	0.1441	0.00386	0.046705
5	0.18885	0.08592	0.07822	0.002095	0.02535
2.5	0.1281	0.05825	0.05303	0.00142	0.01719
1	0.069695	0.031705	0.028865	0.000773	0.009355

IV) Based on criterion for BIOTA (body burden) :

% of time	Loading (kg/day), for outfall:				
exceeded	Dom/CIL	Court–VS	Court–A	Court–S	WPCP
99	−0.00374	−0.0017	−0.00155	−4.2E−05	−0.0005
97.5	−0.00565	−0.00257	−0.00234	−6.3E−05	−0.00076
95	−0.00707	−0.00322	−0.00293	−7.8E−05	−0.00095
90	−0.00781	−0.00355	−0.00323	−8.7E−05	−0.00105
80	−0.00873	−0.00397	−0.00362	−9.7E−05	−0.00117
75	−0.009	−0.00409	−0.00373	−1.0E−04	−0.00121
50	−0.01026	−0.00467	−0.00425	−0.00011	−0.00138
25	−0.01107	−0.00504	−0.00458	−0.00012	−0.00149
20	−0.01123	−0.00511	−0.00465	−0.00012	−0.00151
10	−0.0116	−0.00528	−0.0048	−0.00013	−0.00156
5	−0.01183	−0.00538	−0.0049	−0.00013	−0.00159
2.5	−0.01205	−0.00548	−0.00499	−0.00013	−0.00162
1	−0.01212	−0.00551	−0.00502	−0.00013	−0.00163

Table 5.5a : Probabilistic loading limits using Case I – For : MERCURY

I) Based on criterion for WATER–COLUMN :

% of time exceeded	Loading (kg/day), for outfall:				
	Dom/CIL	Court–VS	Court–A	Court–S	WPCP
99	10.43	4.7455	4.3205	0.1157	1.4
97.5	8.984	4.087	3.72	0.09964	1.206
95	7.847	3.5695	3.25	0.087035	1.0535
90	7.0425	3.2035	2.9165	0.078105	0.9452
80	5.446	2.477	2.2555	0.060395	0.7309
75	4.948	2.2505	2.049	0.05488	0.6641
50	3.623	1.648	1.5005	0.040185	0.48625
25	2.506	1.14	1.0375	0.027795	0.33635
20	2.2825	1.038	0.9452	0.025315	0.3063
10	1.8775	0.854	0.7775	0.020825	0.25195
5	1.549	0.7046	0.64145	0.01718	0.20785
2.5	1.35	0.6143	0.5592	0.01498	0.1812
1	1.112	0.50575	0.46045	0.012335	0.1492

II) Based on criterion for SEDIMENT (LEL) :

% of time exceeded	Loading (kg/day), for outfall:				
	Dom/CIL	Court–VS	Court–A	Court–S	WPCP
99	57.53	26.17	23.825	0.638	7.721
97.5	31.28	14.23	12.95	0.3469	4.198
95	15.645	7.116	6.4785	0.17355	2.0995
90	6.8335	3.108	2.83	0.075785	0.91715
80	2.7895	1.269	1.155	0.030935	0.3744
75	1.948	0.88625	0.80685	0.02161	0.2615
50	0.52345	0.2381	0.2168	0.005806	0.07026
25	0.1201	0.05462	0.049725	0.001332	0.016115
20	0.078075	0.035515	0.032335	0.000866	0.01048
10	0.033615	0.01529	0.01392	0.000373	0.004512
5	0.013175	0.005994	0.005457	0.000146	0.001769
2.5	0.007239	0.003293	0.002998	0.00008	0.000972
1	0.003582	0.001629	0.001483	0.00004	0.000481

III) Based on criterion for BIOTA (body burden) :

% of time exceeded	Loading (kg/day), for outfall:				
	Dom/CIL	Court–VS	Court–A	Court–S	WPCP
99	21.95	9.989	9.0915	0.24345	2.9465
97.5	19.95	9.076	8.263	0.2213	2.678
95	16.815	7.65	6.965	0.18655	2.257
90	13.17	5.991	5.4545	0.14605	1.768
80	9.606	4.3695	3.978	0.10655	1.289
75	8.4735	3.8545	3.509	0.09398	1.1375
50	5.6795	2.583	2.352	0.062985	0.7622
25	3.6345	1.653	1.505	0.04031	0.4878
20	3.3005	1.501	1.367	0.036605	0.44295
10	2.438	1.109	1.0095	0.02704	0.3272
5	1.8555	0.84405	0.7684	0.020575	0.249
2.5	1.396	0.6351	0.5782	0.01549	0.1874
1	0.91875	0.41795	0.38045	0.01019	0.1233

Table 5.5b : Probabilistic loading limits using Case I – For : ZINC

I) Based on criterion for WATER–COLUMN :

% of time exceeded	Loading (kg/day), for outfall:				
	Dom/CIL	Court–VS	Court–A	Court–S	WPCP
99	1565	711.8	648.05	17.36	210.05
97.5	1348	613	558.1	14.95	180.9
95	1177	535.45	487.45	13.055	158
90	1056.5	480.5	437.5	11.72	141.75
80	816.85	371.55	338.25	9.0595	109.6
75	742.25	337.65	307.4	8.232	99.615
50	543.5	247.25	225.05	6.0275	72.94
25	375.9	171	155.7	4.169	50.45
20	342.35	155.75	141.8	3.797	45.95
10	281.6	128.1	116.6	3.1235	37.795
5	232.35	105.7	96.22	2.577	31.185
2.5	202.6	92.14	83.89	2.247	27.19
1	166.75	75.865	69.06	1.8495	22.38

II) Based on criterion for SEDIMENT (LEL) :

% of time exceeded	Loading (kg/day), for outfall:				
	Dom/CIL	Court–VS	Court–A	Court–S	WPCP
99	986.7	448.85	408.6	10.945	132.4
97.5	573.8	261	237.6	6.364	77.01
95	382.8	174.15	158.5	4.246	51.38
90	286.05	130.15	118.45	3.173	38.395
80	200	90.96	82.81	2.2175	26.84
75	171.4	77.955	70.965	1.901	23
50	89.08	40.52	36.89	0.98795	11.955
25	47.57	21.64	19.7	0.5276	6.3845
20	39.58	18	16.39	0.43895	5.312
10	23.22	10.565	9.6155	0.2575	3.116
5	16.43	7.473	6.8035	0.1822	2.2045
2.5	12.7	5.778	5.26	0.1409	1.705
1	9.8775	4.493	4.0905	0.10955	1.3255

III) Based on criterion for BIOTA (body burden) :

% of time exceeded	Loading (kg/day), for outfall:				
	Dom/CIL	Court–VS	Court–A	Court–S	WPCP
99	8.3405	3.794	3.454	0.092505	1.1195
97.5	7.355	3.346	3.046	0.08157	0.9871
95	6.1015	2.7755	2.5265	0.06767	0.8189
90	5.092	2.3165	2.1085	0.056475	0.6834
80	3.8765	1.7635	1.605	0.04299	0.52025
75	3.4265	1.5585	1.419	0.038005	0.45995
50	2.271	1.033	0.9406	0.025195	0.30485
25	1.515	0.6892	0.62745	0.016805	0.20335
20	1.3115	0.59645	0.543	0.014545	0.17595
10	0.96615	0.4395	0.4001	0.010715	0.1297
5	0.7663	0.3486	0.31735	0.008499	0.10285
2.5	0.594	0.2702	0.246	0.006588	0.07973
1	0.48955	0.22265	0.2027	0.00543	0.065705

Table 5.5c : Probabilistic loading limits using Case I – For : PCBs

I) Based on criterion for WATER–COLUMN :

% of time	Loading (kg/day), for outfall:				
exceeded	Dom/CIL	Court–VS	Court–A	Court–S	WPCP
99	0.05216	0.023725	0.0216	0.000579	0.007001
97.5	0.04492	0.02043	0.0186	0.000498	0.006029
95	0.039235	0.01785	0.01625	0.000435	0.005266
90	0.035215	0.01602	0.014585	0.000391	0.004726
80	0.02723	0.012385	0.011275	0.000302	0.003655
75	0.02474	0.011255	0.01025	0.000274	0.003321
50	0.01812	0.008241	0.007502	0.000201	0.002432
25	0.01253	0.0057	0.005189	0.000139	0.001682
20	0.011415	0.005191	0.004726	0.000127	0.001532
10	0.009387	0.00427	0.003887	0.000104	0.00126
5	0.007745	0.003523	0.003208	0.000086	0.00104
2.5	0.006752	0.003071	0.002796	0.000075	0.000906
1	0.005559	0.002529	0.002302	0.000062	0.000746

II) Based on criterion for SEDIMENT (LEL) :

% of time	Loading (kg/day), for outfall:				
exceeded	Dom/CIL	Court–VS	Court–A	Court–S	WPCP
99	1.291	0.5874	0.5348	0.01432	0.17335
97.5	0.6727	0.306	0.2786	0.007461	0.09028
95	0.38615	0.17565	0.15995	0.004283	0.051825
90	0.2061	0.09376	0.08536	0.002286	0.027665
80	0.093605	0.04258	0.038765	0.001038	0.01256
75	0.06631	0.030165	0.02746	0.000735	0.0089
50	0.01774	0.00807	0.007347	0.000197	0.002381
25	0.005054	0.002299	0.002093	0.000056	0.000678
20	0.003792	0.001725	0.001571	0.000042	0.000509
10	0.001574	0.000716	0.000652	0.000017	0.000211
5	0.00099	0.000451	0.00041	0.000011	0.000133
2.5	0.000686	0.000312	0.000284	7.6E–06	0.000092
1	0.000397	0.000181	0.000165	4.4E–06	0.000053

III) Based on criterion for BIOTA (body burden) :

% of time	Loading (kg/day), for outfall:				
exceeded	Dom/CIL	Court–VS	Court–A	Court–S	WPCP
99	0.01168	0.005314	0.004838	0.00013	0.001568
97.5	0.009564	0.00435	0.003961	0.000106	0.001284
95	0.008349	0.003798	0.003458	0.000093	0.001121
90	0.006666	0.003032	0.002761	0.000074	0.000895
80	0.005564	0.002531	0.002304	0.000062	0.000747
75	0.005195	0.002364	0.002152	0.000058	0.000697
50	0.003785	0.001722	0.001568	0.000042	0.000508
25	0.002641	0.001201	0.001094	0.000029	0.000354
20	0.002431	0.001106	0.001007	0.000027	0.000326
10	0.00192	0.000873	0.000795	0.000021	0.000258
5	0.001597	0.000726	0.000661	0.000018	0.000214
2.5	0.001407	0.00064	0.000583	0.000016	0.000189
1	0.001301	0.000592	0.000539	0.000014	0.000175

b) For meeting the bed sediment and aquatic biota criteria, the limits derived based upon Load Allocation Case IIIb with only model calibration uncertainty are considered. These limits are discussed in Section 5.4.2.

These assumptions are made, based upon the fact that the time scales involved in accumulation of chemicals within both sediment and aquatic biota, are days, weeks or months in duration, whereas the water-column responds virtually instantaneously to all sources of uncertainty.

4) For each parameter / outfall, the most restrictive loading limit obtained from steps 1 through 3 above, (rounded to two significant figures), is taken as the "WQBLL".

5) For parameters for which both sediment impact was modelled and a sediment - SEL criterion is available, (mercury, zinc and PCBs), a "critical impact limit", ("CL"), is also provided. The "CL" is the loading limit corresponding to 5% exceedence (i.e. 95% compliance) of the SEL criterion (again, rounded to two significant figures), considering only model calibration uncertainty.

   The "CL" represents the largest loading rate to avoid excessive in-place impacts, as based upon the SEL. The "CL" is larger than the "WQBLL", and the difference between the two values provides some indication of the sensitivity of the benthic environment (on a chemical concentration basis) immediately downstream of the outfall, due to impact of the specific chemical.

All loading limits involved in these steps, along with the recommended "WQBLL" and "CL" values, are provided in Table 5.6.

It should be noted that the recommended "WQBLL" should only be considered when the existing loading rate exceeds it. Further, the "WQBLL" and "critical loading limit" are only interim values to be considered for parameters that are to be "virtually eliminated" (e.g. PCBs, mercury, B(a)P) according to the long-term MOEE program goals for persistent toxics.

5.6 Comparison of "WQBLLs" to past loading rates

The dischargers in Cornwall fall into 4 MISA-designated sectors, namely: pulp and paper, organic chemical manufacturing, inorganic chemical, and municipal. Comprehensive effluent loading data sets have been collected as part of various MISA monitoring programs. These data were collected during 1987 for the Cornwall WPCP [27], and during 1989-90 for all of the industrial outfalls, [28,29,30].

The recommended "WQBLLs" and "CLs", (provided in Table 5.6) are compared with the average measured loadings obtained from the MISA monitoring reports. This comparison can be used to discern the likely environmental impact of these actual past loadings. This comparison is summarized in Table 5.7.

The information provided in Table 5.7 includes:

i) the actual measured gross loading rates as summarized from the 4 MISA monitoring reports. The total for "Domtar/CIL" include loads from Domtar, ICI and ICI Compac. The total for "Courtaulds - Shorebased" includes loads from all 4 shore-based sewers, (storm, acid recovery, CS2 and Caravelle);

ii) the portions of the gross loads which would be caused by the median, general river background concentrations of the parameters. This is calculated using the measured effluent discharge, (also provided in the table);

iii) the actual net loading, which is the difference between the actual gross loading and the load due to river background concentration;

iv) the mass flux of the parameter passing through the river, under median general river background concentration and flow-rate.

The actual net loadings may be compared with their recommended "WQBLL" and "CL" values, and with loading limits representing different compliance levels from Table 5.6. Based upon these comparisons, the following observations are made:

i) Mercury: The actual net loadings of all outfalls exceed the "WQBLLs" and "CLs", (which are all zero). By referring briefly to Table 5.6, it is seen that the very restrictive limits are dictated in order to meet the 95 % compliance sediment-LEL and SEL criteria. (This in turn is due to the higher degree of uncertainty in the calibration of the sediment model, owing to the relatively large degree of heterogeneity in the measured sediment concentrations). The total of the actual net loadings are however, rather small, when compared with the mass-flux passed through the river under general background conditions (only around 2 %). They would therefore not likely create any large scale problems within the river. The most significant loading would likely have been that of the combined shore-based Courtaulds' sewers, since they exceeded even the 50 % compliance LEL loading limits (see Table 5.6). Therefore, localized mercury problems near these outfalls would be expected under the loading rates measured during the MISA monitoring.

ii) Zinc: Again, the actual zinc loadings measured during the MISA monitoring would exceed the recommended "WQBLL" (of zero) at all outfalls. However, they are less than the "critical impact limit" at all outfalls except the Courtaulds' acid diffuser and (combined) shore-based sewers. At the acid diffuser, the loading slightly exceeded the median (50 % compliance) loading limit. The combined shore-based sewer loadings were even greater than the 99% exceedence loading limit. Therefore severe zinc impact would be expected under the measured loadings obtained from the MISA monitoring program in the near-shore vicinity of the Courtaulds shore-based sewers.

iii) PCBs: Although the actual net loadings measured in the Domtar/CIL and Cornwall WPCP effluents exceed their recommended "WQBLL" of zero, they are quite small when compared with both the "critical impact limit" and river background mass flux. Thus little impact would be expected within the river due to these two sources.

iv) Phenols: It should be noted that only the phenol isomer was measured in the final effluents of Domtar and the Cornwall WPCP. The entire system was dominated by the Domtar phenol loading, which represented about 97 % of all net loads. The Domtar/CIL load exceeded the recommended "WQBLL" by a factor of about 2, but was approximately equivalent to the 50 % compliance loading limit (of 14.6 kg/day). Thus, the 1 ppb criterion would be exceeded approximately 50 % of the time at the ENF just downstream of the Domtar/CIL diffuser, under the loading measured during the MISA monitoring.

For similar reasons, the measured net loading from the shore-based Courtaulds sewers would have exceeded the 1 ppb criterion around 50 % of the time in the immediate vicinity of these outfalls.

v) Suspended solids: The actual measured loadings from the Domtar/CIL, Courtaulds shore-based sewers, and Cornwall WPCP greatly exceed the recommended "WQBLL". However the "WQBLL" are based on a very restrictive, and somewhat arbitrary criterion of only a 10 % increase in the suspended sediment concentration at the ENF locations, (i.e. a mixed concentration of 0.99 mg/L, compared with the assumed median river background of 0.9 mg/L). Under the measured sediment loadings, the mixed suspended sediment concentration at the ENF (under the median river background concentration) would be only about: 2, 4 and 2 mg/L, respectively, for these three outfall locations. In fact the total net loadings from the point sources, represent only about 2 % of the general river background mass flux.

One potentially important impact however, might have been from the shore-based Courtaulds' sewers, since the combination of relatively large sediment loadings would likely have helped contribute to large concentrations of particulate zinc and mercury levels in the near-shore bed sediment in the vicinity of these outfalls. This would have been compounded by the very low river current velocities in this zone, (i.e. large settling and low resuspension velocities for the discharged sediments and their adsorbed heavy metals).

6. EVALUATION AND APPLICABILITY OF THE MODELLING TECHNIQUES

6.1 Technique development requirements

6.1.1 Effort required

In terms of subsequent applications of the models used in this study, to assess impacts along the same stretch of the St. Lawrence River, the following notes are provided:

Table 5.6 : **Comparison of loading limits and recommended "water-quality-based loading limits" (WQBLLs) :**

Parameter	Criterion	% time Exceeded	Net, mean-loading (kg/day), for outfall : Dom/CIL	Court-VS	Court-A	Court-S	WPCP
Mercury	water	50	2.77	1.26	1.15	0.031	0.372
		5	1.19	0.54	0.492	0.013	0.159
	sediment - LEL	50	0.308	0.14	0.128	0.00342	0.0413
		5	0	0	0	0	0
	sediment - SEL	50	4.21	1.92	1.74	0.0467	0.565
		5	0	0	0	0	0
	aquatic biota	50	4.55	2.07	1.88	0.0504	0.61
		5	1.31	0.594	0.541	0.0145	0.175
	Recommended WQBLL *		0	0	0	0	0
	Critical impact limit		0	0	0	0	0
Zinc	water	50	412	187	170	4.56	55.2
		5	175	79.6	72.4	1.94	23.5
	sediment - LEL	50	44.5	20.2	18.4	0.493	5.97
		5	0	0	0	0	0
	sediment - SEL	50	458	208	190	5.08	61.5
		5	62.9	28.6	26	0.697	8.44
	Recommended WQBLL *		0	0	0	0	0
	Critical impact limit		63	29	26	0.7	8.4
PCBs	water	50	0	0	0	0	0
		5	0	0	0	0	0
	sediment - LEL	50	0.0019	0.00086	0.00079	0.00002	0.00025
		5	0	0	0	0	0
	sediment - SEL	50	4	1.82	1.66	0.0444	0.537
		5	0.189	0.0859	0.078	0.0021	0.0254
	aquatic biota	50	0	0	0	0	0
		5	0	0	0	0	0
	Recom'd WQBLL * (g/d)		0	0	0	0	0
	Critical impact limit (g/d)		190	86	78	2.1	25
B(a)P	water	50	0.00088	0.0004	0.00036	9.7E-06	0.00012
		5	0.00038	0.00017	0.00016	4.2E-06	0.00005
	Recom'd WQBLL * (g/d)		0.38	0.17	0.16	0.0042	0.05
Phenols	water	50	14.6	6.64	6.05	0.162	1.96
		5	6.24	2.84	2.58	0.0692	0.838
	Recommended WQBLL *		6.2	2.8	2.6	0.07	0.84
Suspended Solids	water	50	1320	598	545	14.6	177
		5	562	256	233	6.24	75.5
	Recommended WQBLL *		1300	600	550	15	180

NOTE: a "WQBLL" should be considered only if it is less than the existing loading rate.

Table 5.7 : **Comparison of "WQBLLs" to existing outfall and background loading rates**

Parameter	Type of effluent loading	**Mass – flux (kg/day) within :**					
		discharged effluent of outfall :					**u/s river**
		Dom/CIL	Court–VS	Court–A	Court–S	WPCP	**bgrd. :**
Mercury	Actual gross loading	0.06512	0.007	0.056	0.011	0.00193	6.22
	Load due to background	0.00134	0.00002	0.00005	0.00059	0.00048	
	Actual net loading	0.06378	0.00698	0.05595	0.01041	0.00145	
	Recommended WQBLL *	0	0	0	0	0	
	Critical impact limit	0	0	0	0	0	
Zinc	Actual gross loading	5.998	2.93	273.6	68.77	1.45	1244.16
	Load due to background	0.26749	0.00304	0.01085	0.11854	0.0966	
	Actual net loading	5.73051	2.92696	273.589	68.6515	1.3534	
	Recommended WQBLL *	0	0	0	0	0	
	Critical impact limit	63	29	26	0.7	8.4	
PCBs	Actual gross loading (g/d)	0.312				2.42	622
	Load due to backg'd (g/d)	0.13375	0.00152	0.00543	0.05927	0.0483	(g/d)
	Actual net loading (g/d)	0.17825				2.3717	
	Recom'd WQBLL * (g/d)	0	0	0	0	0	
	Critical impact limit (g/d)	190	86	78	2.1	25	
B(a)P	Actual gross loading						0.00
	Load due to background	0	0	0	0	0	(g/d)
	Actual net loading						
	Recom'd WQBLL * (g/d)	0.38	0.17	0.16	0.0042	0.05	
Phenols	Actual gross loading	13.4151	0.044	0.092	0.224	0.0908	0.68
	Load due to background	0.00015	2E–06	6E–06	0.00007	0.00005	
	Actual net loading	13.415	0.044	0.09199	0.22393	0.09075	
	Recommended WQBLL *	6.2	2.8	2.6	0.069	0.84	
Suspended solids	Actual gross loading	9976.1	172	498	521.1	1752	559872
	Load due to background	120.372	1.36858	4.88333	53.3434	43.4678	
	Actual net loading	9855.73	170.631	493.117	467.757	1708.53	
	Recommended WQBLL *	1300	600	550	15	180	
Measured effluent discharge (cms)		1.548	0.0176	0.0628	0.686	0.559	

NOTES:
1. "Actual gross loading" & "effluent discharge" were measured during MISA monitoring (as taken from References [27, 28, 29 and 30]).
2. Loading for Domtar/CIL, include loads from: Domtar, ICI, ICI Compac and Cornwall Chemicals.
3. Loading for "Court–S", includes the loads from all 4 shore–based sewers: storm, acid recovery, CS2 and Caravelle.
4. "Load due to background" is based on median river background concentration (see Table 3.1) and the "measured effluent discharge".
5. "Mass–flux within u/s river bgrd." is that which passes Cornwall within the entire river, based upon median river background concentration and flow–rate.

i) Little effort would be required (in the order of a day or less per chemical), for application of either the "KETOX" or "MULTISOURCE" models to evaluate impacts in the water-column. However this assumes that the behaviour of the chemical within the water is known ahead of time. Some literature review may be necessary to acquire this information.

ii) For chemicals (with strong affinity for sediment and biota), and not considered in the current study: Calibration of the partitioning behaviour of these chemicals would have to be performed before applying the sediment impact model. Likewise, calibration of the chemical uptake efficiencies and chemical partitioning with lipid, would have to be calibrated for application of either the Thomann food chain or foodweb models. Depending upon the chemical, this could take from 1 day to 1 week to perform. In the absence of field data for calibration, a good literature data set might be used for screening purposes only.

To apply the modelling system (i.e. the linked models used to describe impact in the water-column, sediment and biota) to other sites would require considerably more time, likely around 1 or 2 months. About half of this time would be required for applying the "KETOX" or "MULTISOURCE" model, because of the large input data requirement. The "LOTUS 1-2-3" spreadsheets, developed for calibrating the sediment and biota models might be used for application at other sites, by substituting the appropriate field data parameters from the new site into them.

The various load allocation equations, and stochastic procedures (including the computer program), developed in Sections 4 and 5, could be applied at other sites, with no modifications. The various parameters used by these equations are derived from application of the water-column, sediment and biota models. Therefore, these models would have to be applied first.

6.1.2 Resource requirements

The "KETOX" and "MULTISOURCE" models have been developed for use on any level of IBM-compatible PC with a math co-processor (to increase simulation speed). As a "bench mark", maximum simulation times for these models for simulation of the St. Lawrence River in the Cornwall vicinity, are around 5 to 10 minutes, on a 386-25 megahertz PC. If necessary, the source codes for these models could also be compiled for use on PCs which do not have a math co-processor. Simulation times for PCs with no math co-processor would likely be about 3 to 5 times longer.

In addition to the modelling system, the user needs to have data editing software for creating and editing the various data files used by the models. Also, to use the calibration spread-sheets provided in the Appendices, the user would need to have "LOTUS 1-2-3". The user must also have a statistical analysis software package for assessing the stochastic characteristics of the various uncertainty parameters. This package should be able to import/export data between itself, and the other data file formats (e.g. "ASCII" and "LOTUS 1-2-3") in this study.

Staff involved in applications of these models should have expertise in environmental simulation

modelling. They should also have access to other staff with expertise in river mechanics, geochemistry, aquatic biology (especially in regards to aquatic foodwebs), and environmental statistics.

6.2 Utility of the modelling approach

6.2.1 Types of applications

The various models are used to establish a "cause-effect" relationship between effluent loading and the resulting exposure concentrations in the water-column, and accumulated concentrations within the bed sediment and/or aquatic biota. For the current application, this relationship is provided as a function of spatial location, via use of the plume delineation results of the hydrodynamic-dispersion model. The models do not consider the time variable effects introduced by dynamic effluent loading and/or ambient changes to in-place contaminants. (The "KETOX" model does provide an estimate of the time scales involved for the dynamics of in-place contaminants, which should be used for screening purposes only).

As such, the modelling approach used in this study can be used to:

i) derive "water quality based, loading limits" ("WQBLLs"), for a single, or multiple point source discharge(s), within any given river reach;

ii) evaluate various (hypothetical) effluent contaminant control options, for a single, or multiple point source discharge(s), before they are implemented, (e.g. as part of a receiving water assessment). Simulation models are the only means of quantifying this type of assessment; and

iii) assist in the design of monitoring / surveillance plans. The models could extend the interpretation of existing (limited) field data, by serving as a tool to interpolate exposure / accumulated ambient concentrations between the field measurement points. They can also be used to delineate impacts under existing or modified multiple point source loadings, (i.e. this provides a quantification of the expected contaminant concentration at all downstream locations). This information is necessary to devise an efficient monitoring strategy, particularly in the current climate of fiscal restraint, where monies for field data collection / analysis may be limited.

6.2.2 Model reliability

All scientific activities carried-out by agencies involved in environmental surveillance and regulation, must be assessed for reliability in order to make the correct interpretation of the results obtained. For environmental models, a calibration / verification of the key modelling parameters is carried-out. For this study, sufficient data was available for calibration. A rigorous verification was not possible, due to a lack of additional independent data bases. However, the models were qualitatively verified by comparisons of their calibration parameters

with similar applications made for the St. Clair River MISA Pilot Site modelling study.

The stochastic load allocation scheme devised for this work utilizes information regarding the accuracy (or reliability) of the models, as obtained via the calibrations, to provide stochastic effluent loading limits. These results are important since they provide a direct link between model reliability and model application. They can also be used to assess the relative importance of various modelling parameters, in contributing to uncertainty in the models, and thereby help direct future field monitoring activities (to increase model reliability, if needed).

The reliability of the models, in terms of their application results, are depended upon calibration accuracy, and variability in the river flow-rate and river background concentrations. By reviewing Tables 5.1 and 5.2, it is clear that the reliability of most model parameters are high, (i.e. uncertainty is less than a factor of 3 from median to 95 % values). The uncertainty of the sediment model for mercury and PCBs is much larger, as compared with the other 9 parameters. However, this uncertainty is really a reflection of the high heterogeneity of measured concentrations in the sediment, and not necessarily a direct cause of the sediment model itself. This is seen in the fact that the uncertainty of the sediment model for zinc is relatively small. It is not clear, whether sufficient knowledge regarding the causes of these effects can be acquired through field studies, in order to refine the mathematical algorithms used by the sediment model, to increase model reliability. It is likely that some of this uncertainty for mercury and PCBs is due to the fact that sources of these two contaminants are less localized, as compared with zinc. Thus, the factors contributing to the general heterogeneity of contaminants levels in sediment, would become relatively more discernible for mercury and PCBs, as compared with zinc.

7. CONCLUSIONS AND RECOMMENDATIONS

7.1 Conclusions

The main goals of the study have been met. Namely:

i) Water quality assessment techniques have been successfully developed / applied. These techniques provide a quantitative linkage between contaminant loading from the multiple Cornwall point sources, and exposure / accumulated contaminant concentrations in the receiving water, bed sediment and aquatic biota, along the Cornwall water-front. They may be used to derive stochastic "water quality based loading limits" ("WQBLLs"), for specific contaminants, from multiple point source discharges, simultaneously.

ii) The assessment techniques were used to derive "WQBLLs" and "critical impact limits" ("CLs"), for all key point sources and selected contaminants. These are summarized in Table 5.6. The point sources considered include: the Domtar/CIL diffuser, the Courtaulds acid and viscose-sulphide diffusers and shore based outfalls, and the Cornwall WPCP diffuser. The contaminants selected for analysis included: mercury, zinc, PCBs, benzo(a)pyrene, phenols and suspended solids.

iii) The potential use of the developed assessment techniques at other sites has been briefly evaluated in terms of: the requirement of effort and resources, and the utility of the techniques for meeting various program needs.

In reviewing the various results of this study, the following specific conclusions are made:

1) The simulation accuracy of the water column (hydrodynamic / dispersion) models is relatively high, with progressively decreasing accuracy for the aquatic biota and sediment impact models, respectively. The lower accuracy of the sediment impact model, especially for mercury and PCBs, reflects the high degree of heterogeneity of in-place concentrations, and relatively smaller localized loadings of these contaminants, as compared with zinc.

2) The models selected and applied to derive "water quality based effluent loading limits", ("WQBLLs"), may also be used to delineate point source impact zones and assist in the design of ambient monitoring sampling.

3) In deriving "WQBLLs", it is essential to consider the effects of background concentrations due to both general upstream river conditions, and local upstream point sources. By doing this, significantly lower "WQBLLs" are obtained, particularly for conventionals and metals, and also organic contaminants that are relatively common within the Great Lakes.

4) It is necessary to use a load allocation procedure to simultaneously derive "WQBLLs" for multiple (local) point sources. Two possible methods have been derived and successfully applied in this study.

5) To provide confidence in the modelling applications, it is necessary to employ a stochastic load allocation procedure. The Monte-Carlo method developed in this study is relatively simple, yet useful in quantifying both the overall uncertainty, and relative significance of the individual modelling parameters in contributing to that overall uncertainty.

6) The uncertainty due to model calibration error, is particularly important to consider, in deriving "WQBLLs" based upon sediment impact. This is particularly important where the total loading of local point sources of a contaminant is not large, with respect to the river background loading.

7) The modelling analysis verified that excessive in-place levels (with respect to the "severe effects level" (SEL)) of zinc and mercury in the vicinity of Courtaulds, would have occurred under the large historic loadings from the acid diffuser and shore-based outfalls of this now closed facility.

8) The measured loadings of mercury, from the Domtar / CIL and Cornwall WPCP diffusers, exceeded both the recommended "WQBLL" and "critical impact limit" values for these outfalls. Therefore, some significant exceedences of the mercury SEL would have been expected in the downstream vicinity of these diffusers. However, the mercury loadings

from these diffusers are relatively small with respect to the overall upstream river mass flux of mercury. Therefore, the impact pattern downstream of these two sources would not likely be that discernible.

9) The measured loadings of PCBs from the Domtar / CIL and Cornwall WPCP diffusers, exceeded the recommended "WQBLL" values, but were well under the "critical impact limit" values. Therefore, no significant exceedences of the PCBs SEL would have been expected downstream of these two diffusers.

10) The measured loading of phenols from the Domtar/CIL diffuser exceeded the "WQBLL" (for 95 % compliance), but would be expected to meet the water column criterion 50 % of the time, at the end of the defined "regulatory mixing zone".

7.2 Recommendations

1) In order to minimize impacts upon the sediment and aquatic biota downstream of the Cornwall point sources, it is recommended that the "WQBLLs" for mercury be implemented, (i.e. zero net loadings), as a high priority.

2) It is recommended that the "WQBLLs" for zinc, PCBs, phenols and suspended solids be implemented at the Domtar/CIL and Cornwall WPCP diffusers, where possible.

3) In order to improve the sediment model accuracy, it is recommended that more study regarding the mechanisms responsible for accumulation of contaminants in sediment, in terms of explaining the highly heterogeneity found in field measurements, be conducted.

4) It is recommended that a user friendly software package to house the various assessment techniques developed for this study should be developed. This tool could be used for "screening" large numbers of point source discharges to the Connecting Channels of the Great Lakes.

5) The number of measurements for estimating general river background concentrations of the various contaminants considered in this study were very limited. In fact no data was available for benzo(a)pyrene, and very crude data available for mercury. It is recommended that in future surveillance studies, more emphasis be placed on quantifying the true, general river background concentrations for key contaminants, (which are widely dispersed in the Great Lakes system). It is particularly important to quantify the variability of background concentrations, to reduce the uncertainty of the derived "WQBLLs". This information would also be very useful for estimating contaminant fate and transport on a larger scale within the Great Lakes' basin and individual watersheds.

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APPENDIX I

Mathematical description of the "sediment impact model"

The following is a brief mathematical outline of the "sediment impact model", discussed in Section 2.3. This model is used to establish a relationship, between the total contaminant concentration in the water-column, with the particulate contaminant concentration in the bed sediment layer, under steady-state conditions.

The general equation relating the total contaminant concentrations in the water column and bed layers, is as follows:

$$C_{T2} = C_{T1} * \left(\frac{w_a * f_{p1} + k_1 * f_{d1}}{h_2 * K_2 + w_{rs} * f_{p2} + k_1 * f_{d2} + w_s * f_{p2}} \right) \qquad \ldots\ 2.1$$

where:

C_{T2} = *the total contaminant concentration in the bed layer, [e.g. in ug/L]*

C_{T1} = *the total contaminant concentration in the water column, [e.g. in ug/L]*

w_a = *the settling velocity of suspended solids from the water column to the bed layer, [e.g. in m/s]*

w_{rs} = *the resuspension velocity of settled solids from the bed layer into the water column, [e.g. in m/s]*

w_s = *the sedimentation velocity of settled solids from the bed layer into deeper sediment layers, [e.g. in m/s]*

k_1 = *the diffusion exchange coefficient between the water column and bed layer [e.g. in m/s]*

k_2 = *the total transformation loss rate of contaminant within the bed layer [e.g. in 1/s]*

H_2 = *the bed layer thickness [e.g. in m].*

The remaining parameters represent the fraction of contaminant in "dissolved" and "particulate" forms, within the water column and sediment layer. They are obtained, knowing the partitioning coefficients, via the following equations:

$$f_{d1} = \frac{1}{1 + m_1 * PC_1} \qquad \ldots\ 2.2a$$

$$f_{d2} = \frac{1}{1 + \left(\dfrac{m_2 * PC_2}{POR}\right)} \qquad \ldots\ 2.2b$$

$$f_{p1} = \frac{m_1 * PC_1}{1 + m_1 * PC_1} \qquad \ldots\ 2.2c$$

$$f_{p2} = \frac{\left(\dfrac{m_2 * PC_2}{POR}\right)}{1 + \left(\dfrac{m_2 * PC_2}{POR}\right)} \qquad \ldots\ 2.2d$$

where: m_1 = *the suspended sediment concentration in the water column, [e.g.* kg_{solids} / L_{total}*]*

m_2 = *the sediment concentration in the bed layer, [e.g.* kg_{solids} / L_{total}*]*

POR = *the porosity of the bed layer, [e.g.* L_{water} / L_{total}*], and*

PC_1, PC_2 = *the partitioning coefficient of the contaminant in the water column and bed layer, respectively, [e.g. in* $L_{water} / kg_{sediment}$*].*

By definition, the particulate contaminant concentration in the bed layer, "r_2", is defined as follows:

$$r_2 = \frac{C_{D2} * PC_2}{POR} \qquad \ldots\ 2.3$$

where: C_{D2} = *the dissolved contaminant concentration in the bed layer, [e.g. in* $mg_{contaminant} / L_{total}$*]*

$$C_{D2} = f_{d2} * C_{T2} \qquad \ldots\ 2.3b$$

By substituting Eqs. 2.3b and 2.1 into Eq. 2.3, an expression relating the particulate contaminant concentration in the bed to the total contaminant concentration in the water column is obtained, as follows:

$$r_2 = C_{T1} * \left(\frac{f_{d2} * PC_2}{POR}\right) * \left(\frac{w_a * f_{p1} + k_1 * f_{d1}}{h_2 * K_2 + w_{rs} * f_{p2} + k_1 * f_{d2} + w_s * f_{p2}}\right) \qquad \ldots\ 2.4$$

This equation can be rearranged to solve for the total contaminant concentration in the water column which will produce (or is equivalent to) a particulate contaminant concentration in the bed sediment, called "C_{T1eq}", as follows:

$$C_{T1eq} = \frac{r_2}{\left(\frac{f_{d2} * PC_2}{POR}\right) * \left(\frac{w_a * f_{p1} + k_1 * f_{d1}}{h_2 * K_2 + w_{rs} * f_{p2} + k_1 * f_{d2} + w_s * f_{p2}}\right)} \qquad \ldots\ 2.5$$

where: r_2 = *the particulate contaminant concentration in the bed sediment, [e.g. in $mg_{contaminant} / kg_{sediment}$]*

APPENDIX II

Mathematical description of the "Thomann food chain model"

The following is a brief mathematical outline of the "Thomann food chain model", discussed in Section 2.4. This model is used to establish a relationship, between the accumulated contaminant concentrations in 4 aquatic biota trophic levels, and the bioavailable contaminant concentration in the water-column, under steady-state conditions.

The dynamic equation incorporating the various processes considered in the model (i.e. uptake of chemical through respiration; uptake of chemical via food consumption; and reduction of chemical concentration due to chemical excretion and animal growth), is:

$$\frac{dv_i}{dt} = ku_i * c_w + \alpha_{i,i-1} * C_{i,i-1} * v_{i-1} - (K_i + G_i) * v_i \qquad \ldots\ 2.10$$

where:

v = *chemical concentration in the organism, on a lipid-specific basis, [e.g. ug/kg_{lipid}]*

c_w = *bioavailable concentration in the water-column, [e.g. in ug/L_{water}]*

ku = *lipid-specific, uptake rate of the chemical from the water, [e.g. in L_{water}/(kg_{lipid}*day)]*

α = *chemical assimilation efficiency, [e.g. ug absorbed / ug ingested]*

C = *lipid-specific, food consumption rate, [e.g. in kg_{lipid}/(kg_{lipid}*day)]*

K = *chemical excretion rate, [e.g. in day^{-1}]*

G = *net relative growth rate, [e.g. in day^{-1}], and*

i & i-1 = *the relative trophic levels of the predator and prey, respectively, [i.e. where i equals 2, 3 or 4].*

An equation for the food consumption rate, "C", as follows, is derived by assuming a steady-state lipid fraction.

$$C = \frac{G + r}{a} \qquad \ldots\ 2.11$$

where:

G = *net relative growth rate, i.e. the change of organism weight with time, "(dw/dt)/w", [e.g. in day^{-1}]*

r = *relative respiration rate of the organism, [e.g. in day^{-1}], and*

a = *food assimilation efficiency, i.e.fraction of: food energy assimilated / food energy consumed.*

General empirical expressions for the relative growth and respiration rates, "G" and "r", are as follows:

$$G = \delta * w^{-\beta} \qquad \text{... 2.12}$$

$$r = \phi * w^{-\gamma} \qquad \text{... 2.13}$$

where: w = *wet weight of the organism, [in grams], and*

δ, β, Φ, γ *are laboratory measured values.*

The uptake rate of the chemical from the water, "ku", is described by the following empirical equation:

$$ku = 1000 * \left(\frac{w^{-\gamma}}{f_L} \right) * E \qquad \text{... 2.14}$$

where: f_L = *lipid mass fraction of the organism, [e.g. in* g_{lipid} / g_{wet} *]*

E = *efficiency of transfer of the chemical, [i.e. fraction of the chemical transfer efficiency to the oxygen transfer efficiency fraction]*

The chemical excretion rate, "K", is set proportional to the uptake rate, "ku", as follows:

$$K = \frac{ku}{PC_1} \qquad \text{... 2.15}$$

where: PC_l = *the lipid-based, partitioning coefficient, [* L_{water}/kg_{lipid} *].*

The efficiency of transfer of the chemical, "E", is defined via 6 empirical relationships, dependent upon organism weight and chemical "PC_l", (i.e. 2 weight classes and 3 "PC_l" classes). These relationships are as follows:

i) For organism weight less than 50 grams:

$$\textit{for } \log PC_1 \textit{ of } 2 \textit{ to } 5: \quad E = 10^{(-2.6 + 0.5 * \log PC_1)} \qquad \ldots 2.16a$$

$$\textit{for } \log PC_1 \textit{ of } 5 \textit{ to } 6: \quad E = 0.8 \qquad \ldots 2.16b$$

$$\textit{for } \log PC_1 \textit{ of } 6 \textit{ to } 9: \quad E = 10^{(2.9 - 0.5 * \log PC_1)} \qquad \ldots 2.16c$$

ii) For organism weight more than 50 grams:

$$\textit{for } \log PC_1 \textit{ of } 2 \textit{ to } 3: \quad E = 10^{(-1.5 + 0.4 * \log PC_1)} \qquad \ldots 2.16d$$

$$\textit{for } \log PC_1 \textit{ of } 3 \textit{ to } 6: \quad E = 0.5 \qquad \ldots 2.16e$$

$$\textit{for } \log PC_1 \textit{ of } 6 \textit{ to } 9: \quad E = 10^{(1.2 - 0.25 * \log PC_1)} \qquad \ldots 2.16f$$

The bioconcentration factor, "BCF", represents the ratio of chemical concentration in the organism (due only to respiration of bioavailable chemical from the water), to the chemical concentration in the water. The model assumes that at equilibrium, the "BCF", (or "Nw"), is equivalent to the partitioning coefficient, "PC_1". This relationship is used to describe the "BCF" for the lowest trophic level, i.e. phytoplankton. That is:

$$Nw_1 = PC_1 \qquad \ldots 2.17$$

The "field BCF" for the upper three trophic levels, must be corrected for organism growth. Using Eq. 2.12, the following general expression is derived to describe the "field BCF":

$$\ldots\ 2.18$$

The bioaccumulation factor, "BAF", is the ratio of chemical concentration within the organism (due to both respiration and food consumption), to the chemical concentration in the water. It has units of "L_w / kg_{lipid}". The bioaccumulation factor, for trophic levels 2 through 4, is derived from the steady-state version of Eq. 2.10 as follows:

$$BAF_i \equiv N_i = \frac{v_i}{c} = Nw_i * c_w + f_{i,i-1} * v_{i-1} \qquad \ldots\ 2.19$$

where: $f_{i,i-1}$ = *accumulation factor due to food consumption,*

$$f_{i,i-1} = \frac{\alpha_{i,i-1} * C_{i,i-1}}{K_i + G_i} \qquad \ldots\ 2.20$$

Equations 2.18 through 2.20 are used to derive the following "BAF" equations:

$$N_2 = Nw_2 + f_{2,1} * Nw_1 \qquad \ldots\ 2.21a$$

$$N_3 = Nw_3 + f_{3,2} * Nw_2 + f_{3,2} * f_{2,1} * Nw_1 \qquad \ldots\ 2.21b$$

$$N_4 = Nw_4 + f_{4,3} * Nw_3 + f_{4,3} * f_{3,2} * Nw_2 + f_{4,3} * f_{3,2} * f_{2,1} * Nw_1 \qquad \ldots\ 2.21c$$

Equations 2.17 and 2.21, are used to obtain the final chemical concentrations in the organisms, on a "wet-weight" basis, "v_{ww}", using the following equation:

$$vww_i = N_i * c_w * f_{L,i} \qquad \ldots\ 2.22$$

APPENDIX III

Mathematical description of the "Thomann foodweb model"

The following is a brief mathematical outline of the "Thomann foodweb model", discussed in Section 2.5. This model is used to establish a relationship, between the accumulated contaminant concentrations in 5 aquatic biota compartments (including a benthic invertebrate compartment), and the bioavailable contaminant concentrations in the water-column and bed sediment, under steady-state conditions.

The dynamic (time variable) equation incorporating the various processes considered in the model (i.e. uptake of chemical through respiration; uptake of chemical via food consumption; and reduction of chemical concentration due to chemical excretion and animal growth), are:

i) for benthic invertebrates, (i.e. Compartment No. 5):

$$\frac{dv_5}{dt} = ku_5 * (b_{5s} * c_s + b_{5w} * c_w) + p_{5s} * \alpha_{5s} * C_{Loc,5} * r_s + p_{51} * \alpha_{51} * C_{L,5} * v_1 - (K_5 + G_5) * v_5 \qquad \ldots\ 2.23$$

where: b_{5s}, b_{5w} = *fractions of ventilation volumes the benthic organism takes from porewater and water column, respectively, (with:* $b_{5s} + b_{5w} = 1$*),*

p_{5s}, p_{51} = *fractions of consumption mass the benthic organism takes from the bed sediment and water column, respectively, (with:* $p_{5s} + p_{51} = 1$*),*

$C_{Loc,5}$ = *specific feeding rate of sediment, [e.g. in* $g_{organic\ carbon}/(g_{lipid}*day)$*],*

$C_{L,5}$ = *specific feeding rate of phytoplankton / detritus material, [e.g. in* $g_{lipid}/(g_{lipid}*day)$ *], and*

all other parameters, as defined in Section 2.4.1.

ii) for forage fish, (i.e. Compartment No. 3):

$$\frac{dv_3}{dt} = ku_3 * c_w + p_{32} * \alpha_{32} * C_{L,3} * v_2 + p_{35} * \alpha_{35} * C_{L,3} * v_5 - (K_3 + G_3) * v_3 \qquad \ldots\ 2.24$$

where: p_{32}, p_{35} = *fractions of consumption mass the forage fish obtain from zooplankton and benthic invertebrate, respectively, (with:*

$p_{32} + p_{35} = 1$),

$C_{L,3}$ = *general feeding rate for forage fish, [e.g. in $g_{lipid}/(g_{lipid}$*day)], and*

all other parameters, as defined in Section 2.4.1.

A more general form of Equation 2.14 is used to describe the chemical uptake rate from water (across the gill membrane), "ku", [18,24], as follows:

$$ku = \left(\frac{a_{oc} * a_c * r}{a_{wd} * f_L * O_2} \right) * E \qquad \ldots\ 2.25$$

where: a_{oc} = *oxygen to carbon ratio,*

a_c = *carbon to dry weight ratio,*

a_{wd} = *wet to dry ratio,*

O_2 = *oxygen concentration in the water, and*

r, f_L *and* E, *are as described in Section 2.4.1.*

The chemical excretion rate, "K", is also modified to include a loss term for "non gill-membrane" chemical losses such as via fecal material and metabolism. This is done by introducing a term, "K_1", to the Eq. 2.15, as follows:

$$K = \frac{ku}{PC_1} + K_1 \qquad \ldots\ 2.26$$

The food consumption equations are derived through a more detailed analysis of energy usage rates. In the analysis, an assumption is made that the caloric density of all biota dry tissue and sediment organic carbon, are similar. Therefore, the wet to dry weight ratios are introduced into the consumption equations used in the foodweb model.

The foodweb model uses the same growth and respiration equations used for the food chain model, (i.e. Eqs. 2.12 and 2.13). However, they are considered to be based upon "wet weight" for the foodweb model, as opposed to "lipid" for the food chain model.

Based upon the above reasoning, the (lipid) specific consumption equation for biota feeding on biota, becomes:

$$C_{L,i} = \left(\frac{G + r}{a}\right) * \left(\frac{a_{wd,i-1}}{a_{wd,i}}\right) * \left(\frac{f_{L,i-1}}{f_{L,i}}\right) \qquad \dots\ 2.27a$$

where: *all parameters are as defined previously.*

The (lipid) specific consumption equation for biota feeding on sediment organic carbon, is:

$$C_{LOC,i} = \left(\frac{G + r}{a * a_{wd,i}}\right) * \left(\frac{f_{oc,i}}{f_{L,i}}\right) \qquad \dots\ 2.27b$$

where: $f_{oc,i}$ *= the fraction of organic carbon in the predator, and all other parameters are as defined previously.*

The following equations were derived [24] to describe the efficiency of transfer of the chemical (via respiration), "E":

For a "PC_1" of:

2.0 *to* 4.0, $E = 10^{(-2.6 + 0.5 * \log PC_1)}$ ... *2.28a*

4.0 *to* 4.5, $E = 1.1 * \log(PC_1) - 4.15$ ... *2.28b*

4.5 *to* 6.5, $E = 0.8$ ... *2.28c*

6.5 *to* 8.0, $E = -0.4 * \log(PC_1) + 3.4$ ... *2.28d*

8.0 *to* 8.5, $E = -0.3 * \log(PC_1) + 2.6$ ... *2.28e*

$$8.5\ \mathit{to}\ 9.0, \qquad E = -0.08 * \log(PC_1) + 0.73 \qquad \ldots\ 2.28f$$

These equations are applied to all biota regardless of their wet weight, (i.e. no weight classes are used in assigning values of "E"). Also, the chemical assimilation efficiency (via food ingestion), "α", is set equal to the value of "E".

The equations used to describe the field bioconcentration factor in the foodweb model are different to those used by the food chain model (i.e. Eqs. 2.17 and 2.18). For phytoplankton, the "BCF" is set equal to the water column partition coefficient as follows:

... 2.29a

where: f_{ocw} *=fraction of organic carbon in the water column's suspended sediment, and*

m_1 *=suspended sediment concentration in the water column, [e.g. in kg/L].*

For the other biota, the following equation (in general form) is used to obtain the "BCF":

$$Nw = \frac{ku}{G + K} \qquad \ldots\ 2.29b$$

In order to derive the bioaccumulation factors (BAF) for the various biota, the foodweb model uses a few factors not used by the food chain model. These include:

i) The "Biota Sediment Factor" (BSF). This is the ratio of lipid-specific body burden of chemical in an organism, "v", divided by the organic carbon-specific chemical concentration in the bed sediment (which is given by "r_2/f_{ocs}"):

$$BSF_i = \frac{v_i}{\left(\frac{r_2}{f_{ocs}}\right)} \qquad \ldots\ 2.30$$

where: v = $ug_{chemical} / kg_{lipid}$

r_2 = *chemical concentration in the total (dry) bed sediment,*

[in $ug_{chemical}$ / $kg_{sediment}$], and

f_{ocs} *= fraction of organic carbon the (dry) bed sediment.*

ii) Chemical partitioning coefficient between the organic carbon-specific concentration in the bed sediment, to the dissolved concentration in the sediment layer porewater; called "PC_s". Where:

$$PC_s = \frac{\left(\frac{r_2}{f_{ocs}}\right)}{c_s} \qquad \ldots\ 2.31$$

iii) Chemical partitioning coefficient between the organic carbon-specific concentration in the bed sediment, to the dissolved concentration in the water column; called "PC_{ws}". Where:

$$PC_{ws} = \frac{\left(\frac{r_2}{f_{ocs}}\right)}{c_w} \qquad \ldots\ 2.32$$

iv) The "relative water exposure route", called "PC'". Where:

$$PC' = \frac{PC_s * PC_{ws}}{b_{5s} * PC_{ws} + b_{5w} * PC_s} \qquad \ldots\ 2.33$$

v) The "food chain multiplier", called "g". Its generic equation form is as follows:

$$g_{i,j} = \frac{p_{i,j} * \alpha_{i,j} * C_{L,i}}{K_i + G_i} \qquad \ldots\ 2.34$$

where: p_{ij} = *fraction of organism i's diet (food mass), made up of organism j.*

When bed sediment is the food source, "$C_{L,i}$" in Eq. 2.34 is replaced with "$C_{LOC,i}$", and the "food chain multiplier" is designated as "g_{5s}".

Using these factors, the foodweb model derives the "BSF" values (designated with "S_i") for the 5 compartments, sequentially as follows:

i) For benthic invertebrates, (Compartment 5):

$$S_5 = \frac{Nw_5}{PC'} + g_{5,s} + g_{5,1} * \left(\frac{Nw_1}{PC_{ws}}\right) \qquad \ldots\ 2.35a$$

ii) For phytoplankton, (Compartment 1):

$$S_1 = \frac{Nw_1}{PC_{ws}} \qquad \ldots\ 2.35b$$

iii) For zooplankton, (Compartment 2):

$$S_2 = \frac{Nw_2}{PC_{ws}} + g_{2,1} * S_1 \qquad \ldots\ 2.35c$$

iv) For forage fish, (Compartment 3):

$$S_3 = \frac{Nw_3}{PC_{ws}} + g_{3,2} * S_2 + g_{3,5} * S_5 \qquad \ldots\ 2.35d$$

v) For piscivorous fish, (Compartment 4):

$$S_4 = \frac{Nw_4}{PC_{ws}} + g_{4,3} * S_3 \qquad \ldots\ 2.35e$$

As can be seen by observing Eqs. 2.30 and 2.32, the bioaccumulation factor (BAF) for each biota compartment, designated by "N_i", is obtained as follows:

$$N_i = PC_{ws} * S_i \qquad \ldots\ 2.36$$

Finally, the predicted concentrations in each biota compartment, on a "wet-weight" basis, "vww_i", is obtained using the same equation as for the food chain model, (i.e. Eq. 2.22).

APPENDIX IV

Final calibrated "sediment impact model" worksheets for Hg, Zn and PCBs

Cornwall MISA – Loading Limits based upon Sediment protection – For MERCURY

	[1979]	[1985]
River Backgrd Conc: HG [ug/L]	0.24	0.1
: SS [mg/L]	0.9	0.9

Assumed Loading concentrations [kg/day], from Source:

	I	II	III	IV	V
[1979]	1.61	0.017	0.008	0.014	0
[1985]	0.044	0.017	0.008	0.002	0

[1979 Stations]

STN NO.	Bed Seds: Fraction: Sand	Silt	Clay	Fine	TOC mg/g	Conc Sed m1 [mg/L]	m2 [kg/L]	Depth h2 [m]	Poros.	Wa [m/s]	Wrs [m/s]	Ws [m/s]	K2 [1/s]	KL [m/s]	Part Coef PC1 [L/kg]	PC2 [L/kg]	Meas R2 [mg/kg]
106	0.58	0.25	0.16	0.42	94	0.9	0.549	0.03	0.4	9.75E−05	1.57E−10	3.17E−12	0.00E+00	6.10E−06	23900	2577.9	18
105	0.4	0.52	0.07	0.58	57	0.9	0.549	0.03	0.4	9.75E−05	1.57E−10	3.17E−12	0.00E+00	6.10E−06	23900	6001.3	8
104	0.82	0.13	0	0.13	37.5	0.9	0.549	0.03	0.4	9.75E−05	1.57E−10	3.17E−12	0.00E+00	6.10E−06	23900	125.63	1.5
103	0.66	0.24	0.08	0.32	19	0.9	0.549	0.03	0.4	9.75E−05	1.57E−10	3.17E−12	0.00E+00	6.10E−06	23900	1262.1	1.7
101	0.47	0.25	0.07	0.32	12.5	0.9	0.549	0.03	0.4	9.75E−05	1.57E−10	3.17E−12	0.00E+00	6.10E−06	23900	1313.7	2.3
100	0.37	0.02	0	0.02	3.1	0.9	0.549	0.03	0.4	9.75E−05	1.57E−10	3.17E−12	0.00E+00	6.10E−06	23900	1.57	0.2
98	0.74	0.18	0.07	0.25	28	0.9	0.549	0.03	0.4	9.75E−05	1.57E−10	3.17E−12	0.00E+00	6.10E−06	23900	693.97	1.3
95	0.42	0.52	0.07	0.59	48	0.9	0.549	0.03	0.4	9.75E−05	1.57E−10	3.17E−12	0.00E+00	6.10E−06	23900	6080.6	7
94	0.49	0.33	0.14	0.47	35	0.9	0.549	0.03	0.4	9.75E−05	1.57E−10	3.17E−12	0.00E+00	6.10E−06	23900	3458.6	15
90	0.42	0.45	0.07	0.52	28	0.9	0.549	0.03	0.4	9.75E−05	1.57E−10	3.17E−12	0.00E+00	6.10E−06	23900	4479.4	1.5
89	0.15	0.8	0.04	0.84	40	0.9	0.549	0.03	0.4	9.75E−05	1.57E−10	3.17E−12	0.00E+00	6.10E−06	23900	15267	2
88	0.51	0.41	0.07	0.47	31.3	0.9	0.549	0.03	0.4	9.75E−05	1.57E−10	3.17E−12	0.00E+00	6.10E−06	23900	3534.4	0.18
87	0.39	0.53	0.07	0.61	50	0.9	0.549	0.03	0.4	9.75E−05	1.57E−10	3.17E−12	0.00E+00	6.10E−06	23900	6625.5	0.2
93	0.51	0.49	0	0.49	28	0.9	0.549	0.03	0.4	9.75E−05	1.57E−10	3.17E−12	0.00E+00	6.10E−06	23900	3807.7	0.25
92	0.3	0.55	0.13	0.68	70	0.9	0.549	0.03	0.4	9.75E−05	1.57E−10	3.17E−12	0.00E+00	6.10E−06	23900	9029.7	0.18
91	0.71	0.26	0.02	0.28	47	0.9	0.549	0.03	0.4	9.75E−05	1.57E−10	3.17E−12	0.00E+00	6.10E−06	23900	952.38	0.5
71	0.39	0.58	0.02	0.6	49	0.9	0.549	0.03	0.4	9.75E−05	1.57E−10	3.17E−12	0.00E+00	6.10E−06	23900	6569.7	2
63	0.87	0.11	0.01	0.12	9	0.9	0.549	0.03	0.4	9.75E−05	1.57E−10	3.17E−12	0.00E+00	6.10E−06	23900	104.3	0.3

[1985 Stations]

STN NO.	Sand	Silt	Clay	Fine	TOC mg/g	m1 [mg/L]	m2 [kg/L]	h2 [m]	Poros.	Wa [m/s]	Wrs [m/s]	Ws [m/s]	K2 [1/s]	KL [m/s]	PC1 [L/kg]	PC2 [L/kg]	Meas R2 [mg/kg]
362	0.89	0.08	0.01	0.09		0.9	0.549	0.03	0.4	9.75E−05	1.57E−10	3.17E−12	0.00E+00	6.10E−06	23900	46.88	0.03
365	0.33	0.52	0.14	0.66		0.9	0.549	0.03	0.4	9.75E−05	1.57E−10	3.17E−12	0.00E+00	6.10E−06	23900	8273.6	0.63
366	0.92	0.06	0.01	0.07		0.9	0.549	0.03	0.4	9.75E−05	1.57E−10	3.17E−12	0.00E+00	6.10E−06	23900	31.013	0.01
3661	0.76	0.19	0.03	0.22		0.9	0.549	0.03	0.4	9.75E−05	1.57E−10	3.17E−12	0.00E+00	6.10E−06	23900	506.56	0.9
368	0.4	0.45	0.13	0.58		0.9	0.549	0.03	0.4	9.75E−05	1.57E−10	3.17E−12	0.00E+00	6.10E−06	23900	5975	4.4
3681	0.87	0.1	0.02	0.12		0.9	0.549	0.03	0.4	9.75E−05	1.57E−10	3.17E−12	0.00E+00	6.10E−06	23900	97.715	0.27
3682	0.37	0.5	0.1	0.6		0.9	0.549	0.03	0.4	9.75E−05	1.57E−10	3.17E−12	0.00E+00	6.10E−06	23900	6486.6	0.13
369	0.76	0.16	0.03	0.18		0.9	0.549	0.03	0.4	9.75E−05	1.57E−10	3.17E−12	0.00E+00	6.10E−06	23900	317.31	0.25
3691	0.48	0.41	0.09	0.5		0.9	0.549	0.03	0.4	9.75E−05	1.57E−10	3.17E−12	0.00E+00	6.10E−06	23900	4135.2	1
370	0.09	0.64	0.24	0.88		0.9	0.549	0.03	0.4	9.75E−05	1.57E−10	3.17E−12	0.00E+00	6.10E−06	23900	17245	1.1
371	0.66	0.26	0.07	0.32		0.9	0.549	0.03	0.4	9.75E−05	1.57E−10	3.17E−12	0.00E+00	6.10E−06	23900	1345.3	0.36
3711	0.95	0.04	0.01	0.04		0.9	0.549	0.03	0.4	9.75E−05	1.57E−10	3.17E−12	0.00E+00	6.10E−06	23900	7.4378	0.12
3712	0.4	0.46	0.1	0.56		0.9	0.549	0.03	0.4	9.75E−05	1.57E−10	3.17E−12	0.00E+00	6.10E−06	23900	5488.8	0.07
3721	0.69	0.25	0.04	0.29		0.9	0.549	0.03	0.4	9.75E−05	1.57E−10	3.17E−12	0.00E+00	6.10E−06	23900	1049.8	0.26
3722	0.3	0.54	0.13	0.67		0.9	0.549	0.03	0.4	9.75E−05	1.57E−10	3.17E−12	0.00E+00	6.10E−06	23900	8696	0.97
373	0.67	0.26	0.06	0.32		0.9	0.549	0.03	0.4	9.75E−05	1.57E−10	3.17E−12	0.00E+00	6.10E−06	23900	1272.3	0.27
3731	0.44	0.46	0.08	0.54		0.9	0.549	0.03	0.4	9.75E−05	1.57E−10	3.17E−12	0.00E+00	6.10E−06	23900	4863.6	0.16
374	0.85	0.12	0.02	0.14		0.9	0.549	0.03	0.4	9.75E−05	1.57E−10	3.17E−12	0.00E+00	6.10E−06	23900	157.93	0.17
3741	0.97	0.03	0.01	0.03		0.9	0.549	0.03	0.4	9.75E−05	1.57E−10	3.17E−12	0.00E+00	6.10E−06	23900	3.4196	0.01
375	0.56	0.34	0.09	0.43		0.9	0.549	0.03	0.4	9.75E−05	1.57E−10	3.17E−12	0.00E+00	6.10E−06	23900	2705.7	0.61
376	0.04	0.63	0.21	0.84		0.9	0.549	0.03	0.4	9.75E−05	1.57E−10	3.17E−12	0.00E+00	6.10E−06	23900	15221	0.77

STN NO.	W.C. Conc:{[ug/L]/[kg/day]}:From: SI	SII	SIII	SIV	SV	W.C. Conc [ug/L] due to LOADING SI	SII	SIII	SIV	SV	W.C. CONC CT1[ug/L]	Fraction Concentration fd1	fd2	fp1	fp2
106	0.03599	0	0	0	0	0.0579	0	0	0	0	0.297944	0.9789	0.0003	0.0211	0.9997
105	0.03525	0	0	0	0	0.0568	0	0	0	0	0.296753	0.9789	0.0001	0.0211	0.9999
104	0.03424	0	0	0	0	0.0551	0	0	0	0	0.295126	0.9789	0.0058	0.0211	0.9942
103	0.03385	0	0	0	0	0.0545	0	0	0	0	0.294499	0.9789	0.0006	0.0211	0.9994
101	0.01478	0	0	0	0	0.0238	0	0	0	0	0.263796	0.9789	0.0006	0.0211	0.9994
100	0.01759	0	0	0	0	0.0283	0	0	0	0	0.26832	0.9789	0.317	0.0211	0.683
98	0.01482	0	0	1.22584	0	0.0239	0	0	0.0172	0	0.281022	0.9789	0.001	0.0211	0.999
95	0.01435	0	0	0.20465	0	0.0231	0	0	0.0029	0	0.265969	0.9789	0.0001	0.0211	0.9999
94	0.01465	0	0	0.55074	0	0.0236	0	0	0.0077	0	0.271297	0.9789	0.0002	0.0211	0.9998
90	0.01465	0	0	0.19015	0	0.0236	0	0	0.0027	0	0.266249	0.9789	0.0002	0.0211	0.9998
89	0.01396	0.00124	0.00163	0.05093	0	0.0225	2E−05	1E−05	0.0007	0	0.263223	0.9789	5E−05	0.0211	1
88	0.00027	0	0	0	0	0.0004	0	0	0	0	0.240435	0.9789	0.0002	0.0211	0.9998
87	0.00078	0	0	0	0	0.0013	0	0	0	0	0.241256	0.9789	0.0001	0.0211	0.9999
93	0.01293	0.00054	0.00066	0.29833	0	0.0208	9E−06	5E−06	0.0042	0	0.265008	0.9789	0.0002	0.0211	0.9998
92	0.00933	0.00722	0.00721	0.01564	0.01064	0.015	0.0001	6E−05	0.0002	0	0.255421	0.9789	8E−05	0.0211	0.9999
91	0.00827	0.00839	0.00833	0.01089	0.01641	0.0133	0.0001	7E−05	0.0002	0	0.253676	0.9789	0.0008	0.0211	0.9992
71	0.01058	0.00474	0.00479	0.02164	0.00491	0.017	8E−05	4E−05	0.0003	0	0.257456	0.9789	0.0001	0.0211	0.9999
63	0.01094	0.00411	0.00419	0.02326	0.00909	0.0176	7E−05	3E−05	0.0003	0	0.258042	0.9789	0.0069	0.0211	0.9931
[1985 Stations]															
362	0	0	0	0	0	0	0	0	0	0	0.1	0.9789	0.0153	0.0211	0.9847
365	0.03344	0	0	0	0	0.0015	0	0	0	0	0.101471	0.9789	9E−05	0.0211	0.9999
366	0.00034	0	0	0	0	1E−05	0	0	0	0	0.100015	0.9789	0.023	0.0211	0.977
3661	0.02393	0	0	0	0	0.0011	0	0	0	0	0.101053	0.9789	0.0014	0.0211	0.9986
368	0.01465	0	0	0.55074	0	0.0006	0	0	0.0011	0	0.101746	0.9789	0.0001	0.0211	0.9999
3681	0.01232	0	0	0	0	0.0005	0	0	0	0	0.100542	0.9789	0.0074	0.0211	0.9926
3682	0.00915	0	0.00387	0	0	0.0004	0	3E−05	0	0	0.100434	0.9789	0.0001	0.0211	0.9999
369	0.01435	0.00009	0.00033	0.74591	0	0.0006	2E−06	3E−06	0.0015	0	0.102127	0.9789	0.0023	0.0211	0.9977
3691	0.01041	0.00205	0.00283	0.02384	0	0.0005	3E−05	2E−05	5E−05	0	0.100563	0.9789	0.0002	0.0211	0.9998
370	0.00994	0.0299	0.00611	0.01877	0	0.0004	0.0005	5E−05	4E−05	0	0.101032	0.9789	4E−05	0.0211	1
371	0.00743	0.00906	0.00895	0.00769	0.0172	0.0003	0.0002	7E−05	2E−05	0	0.100568	0.9789	0.0005	0.0211	0.9995
3711	0.00938	0.00693	0.00693	0.01574	0.00915	0.0004	0.0001	6E−05	3E−05	0	0.100617	0.9789	0.0892	0.0211	0.9108
3712	0.01265	0.00102	0.00106	0.41059	0	0.0006	2E−05	8E−06	0.0008	0	0.101404	0.9789	0.0001	0.0211	0.9999
3721	0.01097	0.00408	0.00416	0.02352	0.0032	0.0005	7E−05	3E−05	5E−05	0	0.100632	0.9789	0.0007	0.0211	0.9993
3722	0.00716	0.00904	0.00894	0.00688	0.01529	0.0003	0.0002	7E−05	1E−05	0	0.100554	0.9789	8E−05	0.0211	0.9999
373	0.01104	0.00493	0.00498	0.0238	0.00542	0.0005	8E−05	4E−05	5E−05	0	0.100657	0.9789	0.0006	0.0211	0.9994
3731	0.00777	0.00802	0.00503	0.00978	0.01157	0.0003	0.0001	4E−05	2E−05	0	0.100538	0.9789	0.0001	0.0211	0.9999
374	0.01083	0.00432	0.0065	0.02262	0.00433	0.0005	7E−05	5E−05	5E−05	0	0.100647	0.9789	0.0046	0.0211	0.9954
3741	0.00586	0.00752	0.00677	0.00521	0.0096	0.0003	0.0001	5E−05	1E−05	0	0.10045	0.9789	0.1756	0.0211	0.8244
375	0.00943	0.0065	0.00659	0.01633	0.00908	0.0004	0.0001	5E−05	3E−05	0	0.100611	0.9789	0.0003	0.0211	0.9997
376	0.01059	0.00471	0.00478	0.02169	0.00486	0.0005	8E−05	4E−05	4E−05	0	0.100628	0.9789	5E−05	0.0211	1

VALUE OF "B" COEFFICIENT USED = 2.553

[PC2 = PC1 * (FRAC FINES) ^ B]

	1979	1979+85	1985
AVG (r2p−r2m)	−0.6793	−0.0968	0.40256
GEO. AVG (r2p/r2m)	0.98922	0.99959	1.00856
AVG (LOG(r2p/r2m))	−0.0047	−0.0002	0.0037
STD (r2p−r2m)	5.38159	3.78798	1.13289
STD (LOG(r2p/r2m))	0.91087	0.81336	0.71931
STD (r2m)	5.11318	3.81428	0.91941
GEO. AVG (r2m)	1.21565	0.51637	0.24787

STN NO.	CT2 [ug/L]	Conc's in Bulk [ug/L] CD1	CD2	CP1	CP2	Pred r1 [mg/kg]	Pred r2 [mg/kg]	Pred. r2/r1	Meas r2 [mg/kg]	r2p/r2m	r2p−r2m	[r2p−r2m]**2	LOG[r2p/r2m]
106	1269.6	0.2917	0.3587	0.0063	1269.2	6.9709	2.3119	0.3317	18	0.1284	−15.688	246.116	−0.8913
105	2645.2	0.2905	0.3211	0.0062	2644.8	6.943	4.8175	0.6939	8	0.6022	−3.1825	10.128	−0.2203
104	67.042	0.2889	0.3866	0.0062	66.655	6.905	0.1214	0.0176	1.5	0.0809	−1.3786	1.90051	−1.0918
103	642.42	0.2883	0.3706	0.0062	642.05	6.8903	1.1695	0.1697	1.7	0.6879	−0.5305	0.28143	−0.1625
101	597.9	0.2582	0.3314	0.0056	597.57	6.172	1.0885	0.1764	2.3	0.4733	−1.2115	1.46779	−0.3249
100	1.1137	0.2627	0.353	0.0057	0.7607	6.2778	0.0014	0.0002	0.2	0.0069	−0.1986	0.03945	−2.1594
98	343.96	0.2751	0.3607	0.0059	343.59	6.575	0.6259	0.0952	1.3	0.4814	−0.6741	0.45447	−0.3175
95	2396.5	0.2604	0.2871	0.0056	2396.2	6.2228	4.3646	0.7014	7	0.6235	−2.6354	6.94533	−0.2052
94	1507.2	0.2656	0.3174	0.0057	1506.9	6.3475	2.7448	0.4324	15	0.183	−12.255	150.19	−0.7376
90	1855	0.2606	0.3017	0.0056	1854.7	6.2293	3.3784	0.5423	1.5	2.2523	1.87838	3.5283	0.35262
89	4684	0.2577	0.2235	0.0055	4683.8	6.1586	8.5315	1.3853	2	4.2657	6.53147	42.6601	0.62999
88	1361.7	0.2354	0.2807	0.0051	1361.4	5.6254	2.4798	0.4408	0.18	13.777	2.29985	5.2893	1.13915
87	2331.1	0.2362	0.2563	0.0051	2330.8	5.6446	4.2455	0.7521	0.2	21.228	4.04554	16.3664	1.3269
93	1602.9	0.2594	0.3067	0.0056	1602.6	6.2003	2.9191	0.4708	0.25	11.677	2.66915	7.12435	1.06732
92	3143.7	0.25	0.2536	0.0054	3143.5	5.976	5.7258	0.9581	0.18	31.81	5.54582	30.7562	1.50257
91	422.15	0.2483	0.3227	0.0053	421.83	5.9352	0.7684	0.1295	0.5	1.5367	0.26835	0.07201	0.18659
71	2470.6	0.252	0.274	0.0054	2470.4	6.0236	4.4998	0.747	2	2.2499	2.49977	6.24886	0.35216
63	48.757	0.2526	0.3382	0.0054	48.419	6.0374	0.0882	0.0146	0.3	0.294	−0.2118	0.04486	−0.5317
[1985 Stations]													
362	8.5829	0.0979	0.1314	0.0021	8.4516	2.3397	0.0154	0.0066	0.03	0.5132	−0.0146	0.00021	−0.2898
365	1168.3	0.0993	0.1029	0.0021	1168.2	2.3741	2.1279	0.8963	0.63	3.3777	1.49793	2.24379	0.52862
366	5.7265	0.0979	0.1314	0.0021	5.5951	2.34	0.0102	0.0044	0.01	1.0191	0.00019	4E−08	0.00823
3661	90.916	0.0989	0.1306	0.0021	90.785	2.3643	0.1654	0.0699	0.9	0.1837	−0.7346	0.53969	−0.7358
368	903.66	0.0996	0.1102	0.0021	903.55	2.3805	1.6458	0.6914	4.4	0.374	−2.7542	7.58554	−0.4271
3681	17.811	0.0984	0.1318	0.0021	17.679	2.3524	0.0322	0.0137	0.27	0.1193	−0.2378	0.05655	−0.9235
3682	953.92	0.0983	0.1071	0.0021	953.81	2.3498	1.7374	0.7394	0.13	13.364	1.60736	2.5836	1.12595
369	57.992	0.1	0.1329	0.0022	57.859	2.3894	0.1054	0.0441	0.25	0.4216	−0.1446	0.02091	−0.3751
3691	653.8	0.0984	0.1152	0.0021	653.69	2.3529	1.1907	0.5061	1	1.1907	0.19069	0.03636	0.0758
370	1941.5	0.0989	0.082	0.0021	1941.5	2.3638	3.5364	1.496	1.1	3.2149	2.43635	5.93582	0.50716
371	233.16	0.0985	0.1262	0.0021	233.04	2.353	0.4245	0.1804	0.36	1.1791	0.06448	0.00416	0.07155
3711	1.4834	0.0985	0.1324	0.0021	1.3511	2.3541	0.0025	0.001	0.12	0.0205	−0.1175	0.01382	−1.6881
3712	839.42	0.0993	0.1114	0.0021	839.31	2.3725	1.5288	0.6444	0.07	21.84	1.4588	2.12811	1.33925
3721	183.95	0.0985	0.1276	0.0021	183.82	2.3545	0.3348	0.1422	0.26	1.2878	0.07483	0.0056	0.10986
3722	1202.8	0.0984	0.1008	0.0021	1202.7	2.3526	2.1907	0.9312	0.97	2.2584	1.22069	1.49009	0.35381
373	221.27	0.0985	0.1266	0.0021	221.15	2.355	0.4028	0.171	0.27	1.4919	0.13282	0.01764	0.17375
3731	751.6	0.0984	0.1126	0.0021	751.48	2.3523	1.3688	0.5819	0.16	8.5551	1.20882	1.46125	0.93223
374	28.674	0.0985	0.1317	0.0021	28.542	2.3548	0.052	0.0221	0.17	0.3058	−0.118	0.01393	−0.5145
3741	0.7524	0.0983	0.1321	0.0021	0.6202	2.3502	0.0011	0.0005	0.01	0.113	−0.0089	0.00008	−0.947
375	448.09	0.0985	0.1206	0.0021	447.97	2.354	0.816	0.3466	0.61	1.3377	0.20598	0.04243	0.12635
376	1787.1	0.0985	0.0855	0.0021	1787	2.3544	3.2551	1.3826	0.77	4.2274	2.4851	6.1757	0.62607

Cornwall MISA – Loading Limits based upon Sediment protection – For ZINC

River Backgrd Conc: ZN [ug/L]	4.6	6.1	Assumed Loading concentrations [kg/day], from Source:					
: SS [mg/L]	0.9	0.9		I	II	III	IV	V
	[1979]	[1985]	[1979]	18	33	360	100	5
			[1985]	8	9	180	30	1

[1979 Stations]

STN NO.	Bed Seds: Fraction: Sand	Silt	Clay	Fine	TOC mg/g	Conc Sed m1 [mg/L]	m2 [kg/L]	Depth h2 [m]	Poros.	Wa [m/s]	Wrs [m/s]	Ws [m/s]	K2 [1/s]	KL [m/s]	Part Coef PC1 [L/kg]	PC2 [L/kg]	Meas R2 [mg/kg]
106	0.58	0.25	0.16	0.42	94	0.9	0.549	0.03	0.4	9.75E–05	1.57E–10	3.17E–12	0.00E+00	6.10E–06	17700	9073.9	180
105	0.4	0.52	0.07	0.58	57	0.9	0.549	0.03	0.4	9.75E–05	1.57E–10	3.17E–12	0.00E+00	6.10E–06	17700	11692	120
104	0.82	0.13	0	0.13	37.5	0.9	0.549	0.03	0.4	9.75E–05	1.57E–10	3.17E–12	0.00E+00	6.10E–06	17700	3665.2	50
103	0.66	0.24	0.08	0.32	19	0.9	0.549	0.03	0.4	9.75E–05	1.57E–10	3.17E–12	0.00E+00	6.10E–06	17700	7323.8	60
101	0.47	0.25	0.07	0.32	12.5	0.9	0.549	0.03	0.4	9.75E–05	1.57E–10	3.17E–12	0.00E+00	6.10E–06	17700	7412.4	40
100	0.37	0.02	0	0.02	3.1	0.9	0.549	0.03	0.4	9.75E–05	1.57E–10	3.17E–12	0.00E+00	6.10E–06	17700	984.14	25
98	0.74	0.18	0.07	0.25	28	0.9	0.549	0.03	0.4	9.75E–05	1.57E–10	3.17E–12	0.00E+00	6.10E–06	17700	6120.6	1200
95	0.42	0.52	0.07	0.59	48	0.9	0.549	0.03	0.4	9.75E–05	1.57E–10	3.17E–12	0.00E+00	6.10E–06	17700	11739	1400
94	0.49	0.33	0.14	0.47	35	0.9	0.549	0.03	0.4	9.75E–05	1.57E–10	3.17E–12	0.00E+00	6.10E–06	17700	9910.4	4100
90	0.42	0.45	0.07	0.52	28	0.9	0.549	0.03	0.4	9.75E–05	1.57E–10	3.17E–12	0.00E+00	6.10E–06	17700	10710	300
89	0.15	0.8	0.04	0.84	40	0.9	0.549	0.03	0.4	9.75E–05	1.57E–10	3.17E–12	0.00E+00	6.10E–06	17700	15473	400
88	0.51	0.41	0.07	0.47	31.3	0.9	0.549	0.03	0.4	9.75E–05	1.57E–10	3.17E–12	0.00E+00	6.10E–06	17700	9975.1	120
87	0.39	0.53	0.07	0.61	50	0.9	0.549	0.03	0.4	9.75E–05	1.57E–10	3.17E–12	0.00E+00	6.10E–06	17700	12045	180
93	0.51	0.49	0	0.49	28	0.9	0.549	0.03	0.4	9.75E–05	1.57E–10	3.17E–12	0.00E+00	6.10E–06	17700	10200	180
92	0.3	0.55	0.13	0.68	70	0.9	0.549	0.03	0.4	9.75E–05	1.57E–10	3.17E–12	0.00E+00	6.10E–06	17700	13217	300
91	0.71	0.26	0.02	0.28	47	0.9	0.549	0.03	0.4	9.75E–05	1.57E–10	3.17E–12	0.00E+00	6.10E–06	17700	6730.4	100
71	0.39	0.58	0.02	0.6	49	0.9	0.549	0.03	0.4	9.75E–05	1.57E–10	3.17E–12	0.00E+00	6.10E–06	17700	12014	350
63	0.87	0.11	0.01	0.12	9	0.9	0.549	0.03	0.4	9.75E–05	1.57E–10	3.17E–12	0.00E+00	6.10E–06	17700	3466.1	90

[1985 Stations]

STN NO.	Sand	Silt	Clay	Fine	TOC mg/g	m1 [mg/L]	m2 [kg/L]	h2 [m]	Poros.	Wa [m/s]	Wrs [m/s]	Ws [m/s]	K2 [1/s]	KL [m/s]	PC1 [L/kg]	PC2 [L/kg]	Meas R2 [mg/kg]
362	0.89	0.08	0.01	0.09		0.9	0.549	0.03	0.4	9.75E–05	1.57E–10	3.17E–12	0.00E+00	6.10E–06	17700	2726.7	30
365	0.33	0.52	0.14	0.66		0.9	0.549	0.03	0.4	9.75E–05	1.57E–10	3.17E–12	0.00E+00	6.10E–06	17700	12875	110
366	0.92	0.06	0.01	0.07		0.9	0.549	0.03	0.4	9.75E–05	1.57E–10	3.17E–12	0.00E+00	6.10E–06	17700	2408.8	19
3661	0.76	0.19	0.03	0.22		0.9	0.549	0.03	0.4	9.75E–05	1.57E–10	3.17E–12	0.00E+00	6.10E–06	17700	5569	58
368	0.4	0.45	0.13	0.58		0.9	0.549	0.03	0.4	9.75E–05	1.57E–10	3.17E–12	0.00E+00	6.10E–06	17700	11677	3800
3681	0.87	0.1	0.02	0.12		0.9	0.549	0.03	0.4	9.75E–05	1.57E–10	3.17E–12	0.00E+00	6.10E–06	17700	3399	130
3682	0.37	0.5	0.1	0.6		0.9	0.549	0.03	0.4	9.75E–05	1.57E–10	3.17E–12	0.00E+00	6.10E–06	17700	11968	88
369	0.76	0.16	0.03	0.18		0.9	0.549	0.03	0.4	9.75E–05	1.57E–10	3.17E–12	0.00E+00	6.10E–06	17700	4839.8	260
3691	0.48	0.41	0.09	0.5		0.9	0.549	0.03	0.4	9.75E–05	1.57E–10	3.17E–12	0.00E+00	6.10E–06	17700	10456	210
370	0.09	0.64	0.24	0.88		0.9	0.549	0.03	0.4	9.75E–05	1.57E–10	3.17E–12	0.00E+00	6.10E–06	17700	16049	460
371	0.66	0.26	0.07	0.32		0.9	0.549	0.03	0.4	9.75E–05	1.57E–10	3.17E–12	0.00E+00	6.10E–06	17700	7465.4	240
3711	0.95	0.04	0.01	0.04		0.9	0.549	0.03	0.4	9.75E–05	1.57E–10	3.17E–12	0.00E+00	6.10E–06	17700	1569.5	28
3712	0.4	0.46	0.1	0.56		0.9	0.549	0.03	0.4	9.75E–05	1.57E–10	3.17E–12	0.00E+00	6.10E–06	17700	11383	74
3721	0.69	0.25	0.04	0.29		0.9	0.549	0.03	0.4	9.75E–05	1.57E–10	3.17E–12	0.00E+00	6.10E–06	17700	6929.9	99
3722	0.3	0.54	0.13	0.67		0.9	0.549	0.03	0.4	9.75E–05	1.57E–10	3.17E–12	0.00E+00	6.10E–06	17700	13069	360
373	0.67	0.26	0.06	0.32		0.9	0.549	0.03	0.4	9.75E–05	1.57E–10	3.17E–12	0.00E+00	6.10E–06	17700	7341.5	240
3731	0.44	0.46	0.08	0.54		0.9	0.549	0.03	0.4	9.75E–05	1.57E–10	3.17E–12	0.00E+00	6.10E–06	17700	10978	75
374	0.85	0.12	0.02	0.14		0.9	0.549	0.03	0.4	9.75E–05	1.57E–10	3.17E–12	0.00E+00	6.10E–06	17700	3925.6	98
3741	0.97	0.03	0.01	0.03		0.9	0.549	0.03	0.4	9.75E–05	1.57E–10	3.17E–12	0.00E+00	6.10E–06	17700	1243.1	30
375	0.56	0.34	0.09	0.43		0.9	0.549	0.03	0.4	9.75E–05	1.57E–10	3.17E–12	0.00E+00	6.10E–06	17700	9206.6	300
376	0.04	0.63	0.21	0.84		0.9	0.549	0.03	0.4	9.75E–05	1.57E–10	3.17E–12	0.00E+00	6.10E–06	17700	15459	520

STN NO.	W.C. Conc:{[ug/L]/[kg/day]}:From: SI	SII	SIII	SIV	SV	W.C. Conc [ug/L] due to LOADING SI	SII	SIII	SIV	SV	W.C. CONC CT1[ug/L]	Fraction Concentration fd1	fd2	fp1	fp2
106	0.03599	0	0	0	0	0.6478	0	0	0	0	5.24782	0.9843	8E−05	0.0157	0.9999
105	0.03525	0	0	0	0	0.6345	0	0	0	0	5.2345	0.9843	6E−05	0.0157	0.9999
104	0.03424	0	0	0	0	0.6163	0	0	0	0	5.21632	0.9843	0.0002	0.0157	0.9998
103	0.03385	0	0	0	0	0.6093	0	0	0	0	5.2093	0.9843	1E−04	0.0157	0.9999
101	0.01478	0	0	0	0	0.266	0	0	0	0	4.86604	0.9843	1E−04	0.0157	0.9999
100	0.01759	0	0	0	0	0.3166	0	0	0	0	4.91662	0.9843	0.0007	0.0157	0.9993
98	0.01482	0	0	1.22584	0	0.2668	0	0	122.58	0	127.4508	0.9843	0.0001	0.0157	0.9999
95	0.01435	0	0	0.20465	0	0.2583	0	0	20.465	0	25.3233	0.9843	6E−05	0.0157	0.9999
94	0.01465	0	0	0.55074	0	0.2637	0	0	55.074	0	59.9377	0.9843	7E−05	0.0157	0.9999
90	0.01465	0	0	0.19015	0	0.2637	0	0	19.015	0	23.8787	0.9843	7E−05	0.0157	0.9999
89	0.01396	0.00124	0.00163	0.05093	0	0.2513	0.0409	0.5868	5.093	0	10.572	0.9843	5E−05	0.0157	1
88	0.00027	0	0	0	0	0.0049	0	0	0	0	4.60486	0.9843	7E−05	0.0157	0.9999
87	0.00078	0	0	0	0	0.014	0	0	0	0	4.61404	0.9843	6E−05	0.0157	0.9999
93	0.01293	0.00054	0.00066	0.29833	0	0.2327	0.0178	0.2376	29.833	0	34.92116	0.9843	7E−05	0.0157	0.9999
92	0.00933	0.00722	0.00721	0.01564	0.01064	0.1679	0.2383	2.5956	1.564	0.0532	9.219	0.9843	6E−05	0.0157	0.9999
91	0.00827	0.00839	0.00833	0.01089	0.01641	0.1489	0.2769	2.9988	1.089	0.0821	9.19558	0.9843	0.0001	0.0157	0.9999
71	0.01058	0.00474	0.00479	0.02164	0.00491	0.1904	0.1564	1.7244	2.164	0.0246	8.85981	0.9843	6E−05	0.0157	0.9999
63	0.01094	0.00411	0.00419	0.02326	0.00909	0.1969	0.1356	1.5084	2.326	0.0455	8.8124	0.9843	0.0002	0.0157	0.9998
[1985 Stations]															
362	0	0	0	0	0	0	0	0	0	0	6.1	0.9843	0.0003	0.0157	0.9997
365	0.03344	0	0	0	0	0.2675	0	0	0	0	6.36752	0.9843	6E−05	0.0157	0.9999
366	0.00034	0	0	0	0	0.0027	0	0	0	0	6.10272	0.9843	0.0003	0.0157	0.9997
3661	0.02393	0	0	0	0	0.1914	0	0	0	0	6.29144	0.9843	0.0001	0.0157	0.9999
368	0.01465	0	0	0.55074	0	0.1172	0	0	16.522	0	22.7394	0.9843	6E−05	0.0157	0.9999
3681	0.01232	0	0	0	0	0.0986	0	0	0	0	6.19856	0.9843	0.0002	0.0157	0.9998
3682	0.00915	0	0.00387	0	0	0.0732	0	0.6966	0	0	6.8698	0.9843	6E−05	0.0157	0.9999
369	0.01435	0.00009	0.00033	0.74591	0	0.1148	0.0008	0.0594	22.377	0	28.65231	0.9843	0.0002	0.0157	0.9998
3691	0.01041	0.00205	0.00283	0.02384	0	0.0833	0.0185	0.5094	0.7152	0	7.42633	0.9843	7E−05	0.0157	0.9999
370	0.00994	0.0299	0.00611	0.01877	0	0.0795	0.2691	1.0998	0.5631	0	8.11152	0.9843	5E−05	0.0157	1
371	0.00743	0.00906	0.00895	0.00769	0.0172	0.0594	0.0815	1.611	0.2307	0.0172	8.09988	0.9843	1E−04	0.0157	0.9999
3711	0.00938	0.00693	0.00693	0.01574	0.00915	0.075	0.0624	1.2474	0.4722	0.0092	7.96616	0.9843	0.0005	0.0157	0.9995
3712	0.01265	0.00102	0.00106	0.41059	0	0.1012	0.0092	0.1908	12.318	0	18.71888	0.9843	6E−05	0.0157	0.9999
3721	0.01097	0.00408	0.00416	0.02352	0.0032	0.0878	0.0367	0.7488	0.7056	0.0032	7.68208	0.9843	0.0001	0.0157	0.9999
3722	0.00716	0.00904	0.00894	0.00688	0.01529	0.0573	0.0814	1.6092	0.2064	0.0153	8.06953	0.9843	6E−05	0.0157	0.9999
373	0.01104	0.00493	0.00498	0.0238	0.00542	0.0883	0.0444	0.8964	0.714	0.0054	7.84851	0.9843	1E−04	0.0157	0.9999
3731	0.00777	0.00802	0.00503	0.00978	0.01157	0.0622	0.0722	0.9054	0.2934	0.0116	7.44471	0.9843	7E−05	0.0157	0.9999
374	0.01083	0.00432	0.0065	0.02262	0.00433	0.0866	0.0389	1.17	0.6786	0.0043	8.07845	0.9843	0.0002	0.0157	0.9998
3741	0.00586	0.00752	0.00677	0.00521	0.0096	0.0469	0.0677	1.2186	0.1563	0.0096	7.59906	0.9843	0.0006	0.0157	0.9994
375	0.00943	0.0065	0.00659	0.01633	0.00908	0.0754	0.0585	1.1862	0.4899	0.0091	7.91912	0.9843	8E−05	0.0157	0.9999
376	0.01059	0.00471	0.00478	0.02169	0.00486	0.0847	0.0424	0.8604	0.6507	0.0049	7.74307	0.9843	5E−05	0.0157	1

VALUE OF "B" COEFFICIENT USED = 0.766

[PC2 = PC1 * (FRAC FINES) ^ B]

	1979	1979+85	1985
AVG (r2p−r2m)	−115.94	−141.35	−163.12
GEO. AVG (r2p/r2m)	1.00615	1.00021	0.99514
AVG (LOG(r2p/r2m))	0.00266	0.00009	−0.0021
STD (r2p−r2m)	706.269	701.683	696.991
STD (LOG(r2p/r2m))	0.26537	0.30453	0.33446
STD (r2m)	946.567	867.51	785.389
GEO. AVG (r2m)	196.839	160.923	135.402

STN NO.	CT2 [ug/L]	Conc's in Bulk [ug/L] CD1	CD2	CP1	CP2	Pred r1 [mg/kg]	Pred r2 [mg/kg]	Pred. r2/r1	Meas r2 [mg/kg]	r2p/r2m	r2p−r2m	[r2p−r2m]**2	LOG[r2p /r2m]
106	60856	5.1655	4.8861	0.0823	60851	91.43	110.84	1.2123	180	0.6158	−69.159	4783.03	−0.2106
105	73030	5.1524	4.5505	0.0821	73025	91.198	133.02	1.4585	120	1.1085	13.0151	169.394	0.04472
104	28639	5.1345	5.692	0.0818	28633	90.881	52.155	0.5739	50	1.0431	2.15535	4.64555	0.01833
103	51189	5.1276	5.092	0.0817	51184	90.759	93.232	1.0272	60	1.5539	33.2317	1104.35	0.19141
101	48273	4.7897	4.7445	0.0763	48268	84.778	87.92	1.0371	40	2.198	47.9201	2296.33	0.34203
100	7927.7	4.8395	5.8649	0.0771	7921.9	85.66	14.43	0.1685	25	0.5772	−10.57	111.733	−0.2387
98	1E+06	125.45	129	1.9985	1E+06	2220.5	1973.9	0.889	1200	1.6449	773.926	598962	0.21615
95	354282	24.926	21.988	0.3971	354260	441.19	645.28	1.4626	1400	0.4609	−754.72	569600	−0.3364
94	742295	58.998	54.568	0.9398	742240	1044.3	1352	1.2947	4100	0.3298	−2748	7551585	−0.4818
90	312945	23.504	21.288	0.3744	312924	416.03	569.99	1.3701	300	1.9	269.989	72894.2	0.27875
89	178128	10.406	8.3873	0.1658	178119	184.19	324.44	1.7615	400	0.8111	−75.557	5708.82	−0.0909
88	57302	4.5327	4.1852	0.0722	57298	80.228	104.37	1.3009	120	0.8697	−15.632	244.347	−0.0606
87	65727	4.5417	3.9756	0.0723	65723	80.388	119.71	1.4892	180	0.6651	−60.287	3634.49	−0.1771
93	441737	34.374	31.55	0.5476	441706	608.41	804.56	1.3224	180	4.4698	624.564	390080	0.65029
92	139986	9.0744	7.7163	0.1446	139978	160.62	254.97	1.5874	300	0.8499	−45.031	2027.77	−0.0706
91	84468	9.0514	9.1431	0.1442	84459	160.21	153.84	0.9603	100	1.5384	53.8414	2898.9	0.18707
71	125984	8.7209	7.6398	0.1389	125976	154.36	229.47	1.4866	350	0.6556	−120.53	14528.7	−0.1834
63	46046	8.6742	9.6772	0.1382	46037	153.53	83.856	0.5462	90	0.9317	−6.1443	37.7526	−0.0307
[1985 Stations]													
362	25684	6.0044	6.8609	0.0956	25677	106.28	46.77	0.4401	30	1.559	16.7701	281.236	0.19285
365	94976	6.2677	5.3745	0.0998	94971	110.94	172.99	1.5593	110	1.5726	62.9893	3967.65	0.19663
366	22939	6.007	6.9363	0.0957	22932	106.32	41.771	0.3929	19	2.1984	22.7705	518.498	0.34212
3661	49485	6.1928	6.4733	0.0987	49478	109.61	90.125	0.8222	58	1.5539	32.1247	1032	0.19142
368	316958	22.383	19.776	0.3566	316938	396.18	577.3	1.4572	3800	0.1519	−3222.7	1E+07	−0.8184
3681	31830	6.1014	6.8215	0.0972	31823	107.99	57.965	0.5367	130	0.4459	−72.035	5188.98	−0.3508
3682	97426	6.7621	5.9306	0.1077	97420	119.69	177.45	1.4826	88	2.0165	89.4505	8001.39	0.30459
369	200234	28.203	30.139	0.4493	200204	499.19	364.67	0.7305	260	1.4026	104.669	10955.7	0.14693
3691	95651	7.3099	6.6646	0.1164	95644	129.38	174.22	1.3465	210	0.8296	−35.785	1280.55	−0.0811
370	139896	7.9843	6.3508	0.1272	139889	141.32	254.81	1.803	460	0.5539	−205.19	42104	−0.2565
371	80807	7.9729	7.8857	0.127	80799	141.12	147.17	1.0429	240	0.6132	−92.826	8616.6	−0.2124
3711	20070	7.8412	9.3131	0.1249	20061	138.79	36.541	0.2633	28	1.305	8.54128	72.9534	0.11563
3712	256263	18.425	16.401	0.2935	256246	326.13	466.75	1.4312	74	6.3075	392.751	154254	0.79985
3721	72239	7.5616	7.5943	0.1205	72232	133.84	131.57	0.983	99	1.329	32.5697	1060.79	0.12352
3722	121596	7.943	6.7787	0.1265	121589	140.59	221.47	1.5753	360	0.6152	−138.53	19189.7	−0.211
373	77271	7.7254	7.6679	0.1231	77264	136.74	140.74	1.0292	240	0.5864	−99.265	9853.47	−0.2318
3731	99316	7.328	6.5912	0.1167	99309	129.71	180.89	1.3946	75	2.4119	105.891	11212.8	0.38236
374	47114	7.9518	8.7427	0.1267	47105	140.75	85.801	0.6096	98	0.8755	−12.199	148.813	−0.0577
3741	15336	7.4799	8.9838	0.1192	15327	132.39	27.919	0.2109	30	0.9306	−2.0813	4.33168	−0.0312
375	92843	7.7949	7.3469	0.1242	92836	137.97	169.1	1.2256	300	0.5637	−130.9	17134.9	−0.249
376	130387	7.6217	6.145	0.1214	130380	134.9	237.49	1.7604	520	0.4567	−282.51	79813.6	−0.3404

Cornwall MISA – Loading Limits based upon Sediment protection – For PCBs

	[1979]	[1985]
River Backgd Conc: PCB [ug/L]	0.0009	0.0017
: SS [mg/L]	0.9	0.9

Assumed Loading concentrations [kg/day], from Source:

	I	II	III	IV	V
[1979]	0.03	0.001	0.00039	0.00015	0.0087
[1985]	0.02	0.001	0.0002	0.0001	0.0008

STN NO.	Bed Seds: Fraction: Sand	Silt	Clay	Fine	TOC mg/g	Conc Sed m1 [mg/L]	m2 [kg/L]	Depth h2 [m]	Poros.	Wa [m/s]	Wrs [m/s]	Ws [m/s]	K2 [1/s]	KL [m/s]	Part Coef PC1 [L/kg]	PC2 [L/kg]	Meas R2 [mg/kg]
[1979 Stations]																	
106	0.58	0.25	0.16	0.42	94	0.9	0.549	0.03	0.4	9.75E−05	1.57E−10	3.17E−12	0.00E+00	6.10E−06	176000	19538	0.07
105	0.4	0.52	0.07	0.58	57	0.9	0.549	0.03	0.4	9.75E−05	1.57E−10	3.17E−12	0.00E+00	6.10E−06	176000	44990	0.06
104	0.82	0.13	0	0.13	37.5	0.9	0.549	0.03	0.4	9.75E−05	1.57E−10	3.17E−12	0.00E+00	6.10E−06	176000	990.11	0.05
103	0.66	0.24	0.08	0.32	19	0.9	0.549	0.03	0.4	9.75E−05	1.57E−10	3.17E−12	0.00E+00	6.10E−06	176000	9654.4	0.105
101	0.47	0.25	0.07	0.32	12.5	0.9	0.549	0.03	0.4	9.75E−05	1.57E−10	3.17E−12	0.00E+00	6.10E−06	176000	10044	0.035
100	0.37	0.02	0	0.02	3.1	0.9	0.549	0.03	0.4	9.75E−05	1.57E−10	3.17E−12	0.00E+00	6.10E−06	176000	13.094	0.01
98	0.74	0.18	0.07	0.25	28	0.9	0.549	0.03	0.4	9.75E−05	1.57E−10	3.17E−12	0.00E+00	6.10E−06	176000	5349.6	0.14
95	0.42	0.52	0.07	0.59	48	0.9	0.549	0.03	0.4	9.75E−05	1.57E−10	3.17E−12	0.00E+00	6.10E−06	176000	45577	0.1
94	0.49	0.33	0.14	0.47	35	0.9	0.549	0.03	0.4	9.75E−05	1.57E−10	3.17E−12	0.00E+00	6.10E−06	176000	26114	2.67
90	0.42	0.45	0.07	0.52	28	0.9	0.549	0.03	0.4	9.75E−05	1.57E−10	3.17E−12	0.00E+00	6.10E−06	176000	33708	0.07
89	0.15	0.8	0.04	0.84	40	0.9	0.549	0.03	0.4	9.75E−05	1.57E−10	3.17E−12	0.00E+00	6.10E−06	176000	113082	0.06
87	0.39	0.53	0.07	0.61	50	0.9	0.549	0.03	0.4	9.75E−05	1.57E−10	3.17E−12	0.00E+00	6.10E−06	176000	49606	0.025
71	0.39	0.58	0.02	0.6	49	0.9	0.549	0.03	0.4	9.75E−05	1.57E−10	3.17E−12	0.00E+00	6.10E−06	176000	49194	0.01
63	0.87	0.11	0.01	0.12	9	0.9	0.549	0.03	0.4	9.75E−05	1.57E−10	3.17E−12	0.00E+00	6.10E−06	176000	823.93	0.01
[1985 Stations]																	
362	0.89	0.08	0.01	0.09		0.9	0.549	0.03	0.4	9.75E−05	1.57E−10	3.17E−12	0.00E+00	6.10E−06	176000	374.2	0.02
365	0.33	0.52	0.14	0.66		0.9	0.549	0.03	0.4	9.75E−05	1.57E−10	3.17E−12	0.00E+00	6.10E−06	176000	61768	0.26
3661	0.76	0.19	0.03	0.22		0.9	0.549	0.03	0.4	9.75E−05	1.57E−10	3.17E−12	0.00E+00	6.10E−06	176000	3920.9	0.06
368	0.4	0.45	0.13	0.58		0.9	0.549	0.03	0.4	9.75E−05	1.57E−10	3.17E−12	0.00E+00	6.10E−06	176000	44796	1.01
3681	0.87	0.1	0.02	0.12		0.9	0.549	0.03	0.4	9.75E−05	1.57E−10	3.17E−12	0.00E+00	6.10E−06	176000	772.59	0.02
3682	0.37	0.5	0.1	0.6		0.9	0.549	0.03	0.4	9.75E−05	1.57E−10	3.17E−12	0.00E+00	6.10E−06	176000	48580	0.045
369	0.76	0.16	0.03	0.18		0.9	0.549	0.03	0.4	9.75E−05	1.57E−10	3.17E−12	0.00E+00	6.10E−06	176000	2470.9	0.085
3691	0.48	0.41	0.09	0.5		0.9	0.549	0.03	0.4	9.75E−05	1.57E−10	3.17E−12	0.00E+00	6.10E−06	176000	31150	0.265
370	0.09	0.64	0.24	0.88		0.9	0.549	0.03	0.4	9.75E−05	1.57E−10	3.17E−12	0.00E+00	6.10E−06	176000	127529	0.245
371	0.66	0.26	0.07	0.32		0.9	0.549	0.03	0.4	9.75E−05	1.57E−10	3.17E−12	0.00E+00	6.10E−06	176000	10282	0.06
3711	0.95	0.04	0.01	0.04		0.9	0.549	0.03	0.4	9.75E−05	1.57E−10	3.17E−12	0.00E+00	6.10E−06	176000	60.798	0.02
3712	0.4	0.46	0.1	0.56		0.9	0.549	0.03	0.4	9.75E−05	1.57E−10	3.17E−12	0.00E+00	6.10E−06	176000	41195	0.04
3721	0.69	0.25	0.04	0.29		0.9	0.549	0.03	0.4	9.75E−05	1.57E−10	3.17E−12	0.00E+00	6.10E−06	176000	8049.1	0.075
3722	0.3	0.54	0.13	0.67		0.9	0.549	0.03	0.4	9.75E−05	1.57E−10	3.17E−12	0.00E+00	6.10E−06	176000	64880	0.075
373	0.67	0.26	0.06	0.32		0.9	0.549	0.03	0.4	9.75E−05	1.57E−10	3.17E−12	0.00E+00	6.10E−06	176000	9731.5	0.02
3731	0.44	0.46	0.08	0.54		0.9	0.549	0.03	0.4	9.75E−05	1.57E−10	3.17E−12	0.00E+00	6.10E−06	176000	36560	0.055
374	0.85	0.12	0.02	0.14		0.9	0.549	0.03	0.4	9.75E−05	1.57E−10	3.17E−12	0.00E+00	6.10E−06	176000	1241	0.02
3741	0.97	0.03	0.01	0.03		0.9	0.549	0.03	0.4	9.75E−05	1.57E−10	3.17E−12	0.00E+00	6.10E−06	176000	28.235	0.02
375	0.56	0.34	0.09	0.43		0.9	0.549	0.03	0.4	9.75E−05	1.57E−10	3.17E−12	0.00E+00	6.10E−06	176000	20494	0.085
376	0.04	0.63	0.21	0.84		0.9	0.549	0.03	0.4	9.75E−05	1.57E−10	3.17E−12	0.00E+00	6.10E−06	176000	112742	0.085

STN NO.	W.C. Conc:{[ug/L]/[kg/day]}:From: SI	SII	SIII	SIV	SV	W.C. Conc [ug/L] due to LOADING SI	SII	SIII	SIV	SV	W.C. CONC CT1[ug/L]	Fraction Concentration fd1	fd2	fp1	fp2
106	0.03599	0	0	0	0	0.0011	0	0	0	0	0.00193	0.8633	4E−05	0.1367	1
105	0.03525	0	0	0	0	0.0011	0	0	0	0	0.001908	0.8633	2E−05	0.1367	1
104	0.03424	0	0	0	0	0.001	0	0	0	0	0.001877	0.8633	0.0007	0.1367	0.9993
103	0.03385	0	0	0	0	0.001	0	0	0	0	0.001866	0.8633	8E−05	0.1367	0.9999
101	0.01478	0	0	0	0	0.0004	0	0	0	0	0.001293	0.8633	7E−05	0.1367	0.9999
100	0.01759	0	0	0	0	0.0005	0	0	0	0	0.001378	0.8633	0.0527	0.1367	0.9473
98	0.01482	0	0	1.22584	0	0.0004	0	0	0.0002	0	0.001478	0.8633	0.0001	0.1367	0.9999
95	0.01435	0	0	0.20465	0	0.0004	0	0	3E−05	0	0.001311	0.8633	2E−05	0.1367	1
94	0.01465	0	0	0.55074	0	0.0004	0	0	8E−05	0	0.001372	0.8633	3E−05	0.1367	1
90	0.01465	0	0	0.19015	0	0.0004	0	0	3E−05	0	0.001318	0.8633	2E−05	0.1367	1
89	0.01396	0.00124	0.00163	0.05093	0	0.0004	1E−06	6E−07	8E−06	0	0.001278	0.8633	6E−06	0.1367	1
87	0.00078	0	0	0	0	2E−05	0	0	0	0	0.000873	0.8633	1E−05	0.1367	1
71	0.01058	0.00474	0.00479	0.02164	0.00491	0.0003	5E−06	2E−06	3E−06	4E−05	0.00122	0.8633	1E−05	0.1367	1
63	0.01094	0.00411	0.00419	0.02326	0.00909	0.0003	4E−06	2E−06	3E−06	8E−05	0.001267	0.8633	0.0009	0.1367	0.9991
[1985 Stations]															
362	0	0	0	0	0	0	0	0	0	0	0.0017	0.8633	0.0019	0.1367	0.9981
365	0.03344	0	0	0	0	0.0007	0	0	0	0	0.002369	0.8633	1E−05	0.1367	1
3661	0.02393	0	0	0	0	0.0005	0	0	0	0	0.002179	0.8633	0.0002	0.1367	0.9998
368	0.01465	0	0	0.55074	0	0.0003	0	0	6E−05	0	0.002048	0.8633	2E−05	0.1367	1
3681	0.01232	0	0	0	0	0.0002	0	0	0	0	0.001946	0.8633	0.0009	0.1367	0.9991
3682	0.00915	0	0.00387	0	0	0.0002	0	8E−07	0	0	0.001884	0.8633	1E−05	0.1367	1
369	0.01435	0.00009	0.00033	0.74591	0	0.0003	9E−08	7E−08	7E−05	0	0.002062	0.8633	0.0003	0.1367	0.9997
3691	0.01041	0.00205	0.00283	0.02384	0	0.0002	2E−06	6E−07	2E−06	0	0.001913	0.8633	2E−05	0.1367	1
370	0.00994	0.0299	0.00611	0.01877	0	0.0002	3E−05	1E−06	2E−06	0	0.001932	0.8633	6E−06	0.1367	1
371	0.00743	0.00906	0.00895	0.00769	0.0172	0.0001	9E−06	2E−06	8E−07	1E−05	0.001874	0.8633	7E−05	0.1367	0.9999
3711	0.00938	0.00693	0.00693	0.01574	0.00915	0.0002	7E−06	1E−06	2E−06	7E−06	0.001905	0.8633	0.0118	0.1367	0.9882
3712	0.01265	0.00102	0.00106	0.41059	0	0.0003	1E−06	2E−07	4E−05	0	0.001995	0.8633	2E−05	0.1367	1
3721	0.01097	0.00408	0.00416	0.02352	0.0032	0.0002	4E−06	8E−07	2E−06	3E−06	0.001929	0.8633	9E−05	0.1367	0.9999
3722	0.00716	0.00904	0.00894	0.00688	0.01529	0.0001	9E−06	2E−06	7E−07	1E−05	0.001867	0.8633	1E−05	0.1367	1
373	0.01104	0.00493	0.00498	0.0238	0.00542	0.0002	5E−06	1E−06	2E−06	4E−06	0.001933	0.8633	7E−05	0.1367	0.9999
3731	0.00777	0.00802	0.00503	0.00978	0.01157	0.0002	8E−06	1E−06	1E−06	9E−06	0.001875	0.8633	2E−05	0.1367	1
374	0.01083	0.00432	0.0065	0.02262	0.00433	0.0002	4E−06	1E−06	2E−06	3E−06	0.001928	0.8633	0.0006	0.1367	0.9994
3741	0.00586	0.00752	0.00677	0.00521	0.0096	0.0001	8E−06	1E−06	5E−07	8E−06	0.001834	0.8633	0.0252	0.1367	0.9748
375	0.00943	0.0065	0.00659	0.01633	0.00908	0.0002	7E−06	1E−06	2E−06	7E−06	0.001905	0.8633	4E−05	0.1367	1
376	0.01059	0.00471	0.00478	0.02169	0.00486	0.0002	5E−06	1E−06	2E−06	4E−06	0.001924	0.8633	6E−06	0.1367	1

VALUE OF "B" COEFFICIENT USED = 2.52

[PC2 = PC1 * FINES ^ B]

	1979	1979+85	1985
AVG (r2p−r2m)	−0.1273	−0.0365	0.02699
GEO. AVG (r2p/r2m)	1.01341	0.99787	0.98713
AVG (LOG(r2p/r2m))	0.00579	−0.0009	−0.0056
STD (r2p−r2m)	0.67062	0.46289	0.19909
STD (LOG(r2p/r2m))	0.78736	0.71397	0.65771
STD (r2m)	0.67391	0.46673	0.21658
GEO. AVG (r2m)	0.05606	0.06062	0.06403

STN NO.	CT2 [ug/L]	Conc's in Bulk [ug/L] CD1	CD2	CP1	CP2	Pred r1 [mg/kg]	Pred r2 [mg/kg]	Pred. r2/r1	Meas r2 [mg/kg]	r2p/r2m	r2p−r2m	[r2p−r2m]**2	LOG[r2p /r2m]
106	92.682	0.0017	0.0035	0.0003	92.679	0.2932	0.1688	0.5758	0.07	2.4116	0.09881	0.00976	0.38231
105	137.18	0.0016	0.0022	0.0003	137.18	0.2898	0.2499	0.8622	0.06	4.1646	0.18987	0.03605	0.61957
104	7.519	0.0016	0.0055	0.0003	7.5135	0.2852	0.0137	0.048	0.05	0.2737	−0.0363	0.00132	−0.5627
103	55.963	0.0016	0.0042	0.0003	55.959	0.2834	0.1019	0.3596	0.105	0.9707	−0.0031	9E−06	−0.0129
101	39.951	0.0011	0.0029	0.0002	39.948	0.1965	0.0728	0.3703	0.035	2.079	0.03776	0.00143	0.31785
100	0.0797	0.0012	0.0042	0.0002	0.0755	0.2093	0.0001	0.0007	0.01	0.0137	−0.0099	0.0001	−1.8617
98	27.771	0.0013	0.0038	0.0002	27.767	0.2246	0.0506	0.2252	0.14	0.3613	−0.0894	0.008	−0.4422
95	94.764	0.0011	0.0015	0.0002	94.763	0.1992	0.1726	0.8664	0.1	1.7261	0.07261	0.00527	0.23706
94	77.336	0.0012	0.0022	0.0002	77.333	0.2085	0.1409	0.6757	2.67	0.0528	−2.5291	6.39654	−1.2777
90	84.049	0.0011	0.0018	0.0002	84.047	0.2003	0.1531	0.7645	0.07	2.187	0.08309	0.0069	0.33985
89	119.38	0.0011	0.0008	0.0002	119.38	0.1942	0.2174	1.1196	0.06	3.6241	0.15745	0.02479	0.5592
87	65.127	0.0008	0.001	0.0001	65.126	0.1327	0.1186	0.894	0.025	4.745	0.09363	0.00877	0.67624
71	90.697	0.0011	0.0013	0.0002	90.695	0.1854	0.1652	0.8913	0.01	16.52	0.1552	0.02409	1.21801
63	4.2467	0.0011	0.0038	0.0002	4.2429	0.1924	0.0077	0.0402	0.01	0.7728	−0.0023	5E−06	−0.1119
[1985 Stations]													
362	2.6329	0.0015	0.0051	0.0002	2.6278	0.2583	0.0048	0.0185	0.02	0.2393	−0.0152	0.00023	−0.621
365	190.07	0.002	0.0022	0.0003	190.07	0.3599	0.3462	0.962	0.26	1.3316	0.08621	0.00743	0.12436
3661	31.345	0.0019	0.0058	0.0003	31.339	0.331	0.0571	0.1725	0.06	0.9514	−0.0029	9E−06	−0.0216
368	147.05	0.0018	0.0024	0.0003	147.05	0.3112	0.2678	0.8608	1.01	0.2652	−0.7422	0.55079	−0.5764
3681	6.131	0.0017	0.0058	0.0003	6.1252	0.2957	0.0112	0.0377	0.02	0.5579	−0.0088	0.00008	−0.2535
3682	139.41	0.0016	0.0021	0.0003	139.41	0.2862	0.2539	0.8872	0.045	5.6429	0.20893	0.04365	0.7515
369	19.592	0.0018	0.0058	0.0003	19.586	0.3132	0.0357	0.1139	0.085	0.4197	−0.0493	0.00243	−0.377
3691	117.64	0.0017	0.0028	0.0003	117.64	0.2907	0.2143	0.7371	0.265	0.8086	−0.0507	0.00257	−0.0923
370	184.53	0.0017	0.0011	0.0003	184.53	0.2935	0.3361	1.1452	0.245	1.3719	0.09112	0.0083	0.13733
371	58.886	0.0016	0.0042	0.0003	58.881	0.2847	0.1073	0.3767	0.06	1.7875	0.04725	0.00223	0.25225
3711	0.4896	0.0016	0.0058	0.0003	0.4838	0.2894	0.0009	0.003	0.02	0.0441	−0.0191	0.00037	−1.356
3712	138.62	0.0017	0.0025	0.0003	138.62	0.3032	0.2525	0.8329	0.04	6.3123	0.21249	0.04515	0.80019
3721	50.414	0.0017	0.0046	0.0003	50.409	0.2931	0.0918	0.3133	0.075	1.2243	0.01682	0.00028	0.08788
3722	152.07	0.0016	0.0017	0.0003	152.06	0.2837	0.277	0.9765	0.075	3.6931	0.20198	0.0408	0.56739
373	58.345	0.0017	0.0044	0.0003	58.34	0.2938	0.1063	0.3618	0.02	5.3133	0.08627	0.00744	0.72537
3731	123.91	0.0016	0.0025	0.0003	123.91	0.2848	0.2257	0.7924	0.055	4.1037	0.1707	0.02914	0.61317
374	9.5937	0.0017	0.0056	0.0003	9.5881	0.2929	0.0175	0.0596	0.02	0.8732	−0.0025	6E−06	−0.0589
3741	0.2222	0.0016	0.0056	0.0003	0.2166	0.2787	0.0004	0.0014	0.02	0.0197	−0.0196	0.00038	−1.7049
375	94.088	0.0016	0.0033	0.0003	94.085	0.2895	0.1714	0.592	0.085	2.0162	0.08637	0.00746	0.30453
376	179.53	0.0017	0.0012	0.0003	179.53	0.2922	0.327	1.1189	0.085	3.8471	0.242	0.05857	0.58514

APPENDIX V

Final calibrated "food chain impact model" worksheets for Hg, Zn and PCBs

THOMANN STEADY-STATE, 4 LEVEL FOOD CHAIN MODEL ASSUME: E = EFACTR * E ASSUME: ALF=E*EFACTR*ALFFTR

FOR MERCURY : ESTIMATED LOG KOW = 4.183 EFACTR= 1 ALFFTR= 1

INPUT VALUES FOR MODEL

STN NO	TROPHIC LEVEL	W (gm)	LIP	A	ALF	BETA	GAM	DEL	FI
[1979]									
112	1	0.0002	0.023	0.1	0.1	0.2	0.2	0.01	0.036
	2	0.016	0.016	0.3	0.3	0.2	0.2	0.01	0.036
	3	1.8	0.036	0.8	0.8	0.2	0.2	0.01	0.036
	4	128	0.092	0.8	0.8	0.2	0.2	0.01	0.036
104	1	0.0002	0.023	0.1	0.1	0.2	0.2	0.01	0.036
	2	0.016	0.016	0.3	0.3	0.2	0.2	0.01	0.036
	3	1.8	0.036	0.8	0.8	0.2	0.2	0.01	0.036
	4	128	0.092	0.8	0.8	0.2	0.2	0.01	0.036
95	1	0.0002	0.023	0.1	0.1	0.2	0.2	0.01	0.036
	2	0.016	0.016	0.3	0.3	0.2	0.2	0.01	0.036
	3	1.8	0.036	0.8	0.8	0.2	0.2	0.01	0.036
	4	128	0.092	0.8	0.8	0.2	0.2	0.01	0.036
71	1	0.0002	0.023	0.1	0.1	0.2	0.2	0.01	0.036
	2	0.0024	0.006	0.3	0.3	0.2	0.2	0.01	0.036
	3	1.8	0.036	0.8	0.8	0.2	0.2	0.01	0.036
	4	128	0.092	0.8	0.8	0.2	0.2	0.01	0.036
[1986]									
366a	1	0.0002	0.023	0.1	0.1	0.2	0.2	0.01	0.036
	2	0.0024	0.006	0.3	0.3	0.2	0.2	0.01	0.036
	3	4	0.04	0.8	0.8	0.2	0.2	0.01	0.036
	4	313	0.045	0.8	0.8	0.2	0.2	0.01	0.036
368	1	0.0002	0.023	0.1	0.1	0.2	0.2	0.01	0.036
	2	0.0024	0.003	0.3	0.3	0.2	0.2	0.01	0.036
	3	4.1	0.04	0.8	0.8	0.2	0.2	0.01	0.036
	4	313	0.045	0.8	0.8	0.2	0.2	0.01	0.036
368b	1	0.0002	0.023	0.1	0.1	0.2	0.2	0.01	0.036
	2	0.0024	0.004	0.3	0.3	0.2	0.2	0.01	0.036
	3	4	0.04	0.8	0.8	0.2	0.2	0.01	0.036
	4	313	0.045	0.8	0.8	0.2	0.2	0.01	0.036
369	1	0.0002	0.023	0.1	0.1	0.2	0.2	0.01	0.036
	2	0.0024	0.007	0.3	0.3	0.2	0.2	0.01	0.036
	3	3.8	0.038	0.8	0.8	0.2	0.2	0.01	0.036
	4	313	0.045	0.8	0.8	0.2	0.2	0.01	0.036
371	1	0.0002	0.023	0.1	0.1	0.2	0.2	0.01	0.036
	2	0.0024	0.006	0.3	0.3	0.2	0.2	0.01	0.036
	3	4.1	0.04	0.8	0.8	0.2	0.2	0.01	0.036
	4	313	0.045	0.8	0.8	0.2	0.2	0.01	0.036
371b	1	0.0002	0.023	0.1	0.1	0.2	0.2	0.01	0.036
	2	0.0024	0.007	0.3	0.3	0.2	0.2	0.01	0.036
	3	3.8	0.038	0.8	0.8	0.2	0.2	0.01	0.036
	4	313	0.045	0.8	0.8	0.2	0.2	0.01	0.036
374	1	0.0002	0.023	0.1	0.1	0.2	0.2	0.01	0.036
	2	0.0089	0.007	0.3	0.3	0.2	0.2	0.01	0.036
	3	4.1	0.04	0.8	0.8	0.2	0.2	0.01	0.036
	4	313	0.045	0.8	0.8	0.2	0.2	0.01	0.036
375	1	0.0002	0.023	0.1	0.1	0.2	0.2	0.01	0.036
	2	0.0024	0.006	0.3	0.3	0.2	0.2	0.01	0.036
	3	3.8	0.038	0.8	0.8	0.2	0.2	0.01	0.036
	4	313	0.045	0.8	0.8	0.2	0.2	0.01	0.036
398a	1	0.0002	0.023	0.1	0.1	0.2	0.2	0.01	0.036
	2	0.0024	0.009	0.3	0.3	0.2	0.2	0.01	0.036
	3	2	0.033	0.8	0.8	0.2	0.2	0.01	0.036
	4	313	0.045	0.8	0.8	0.2	0.2	0.01	0.036

Estimation of the Uptake Efficiency "E":

STN NO	TROPHIC LEVEL	Calculated from Eq. E15A	E15B	E15C	E16A	E16B	E16C	Minimum value from: E15AB	E15BC	E15ABC	E16AB	E16BC	E16ABC	E * EFACTR
[1979]														
112	1	0.3101	0.8	6.4343	1.49	0.5	1.4264	0.3101	0.8	0.3101	0.5	0.5	0.5	0.3101
	2	0.3101	0.8	6.4343	1.49	0.5	1.4264	0.3101	0.8	0.3101	0.5	0.5	0.5	0.3101
	3	0.3101	0.8	6.4343	1.49	0.5	1.4264	0.3101	0.8	0.3101	0.5	0.5	0.5	0.3101
	4	0.3101	0.8	6.4343	1.49	0.5	1.4264	0.3101	0.8	0.3101	0.5	0.5	0.5	0.5
104	1	0.3101	0.8	6.4343	1.49	0.5	1.4264	0.3101	0.8	0.3101	0.5	0.5	0.5	0.3101
	2	0.3101	0.8	6.4343	1.49	0.5	1.4264	0.3101	0.8	0.3101	0.5	0.5	0.5	0.3101
	3	0.3101	0.8	6.4343	1.49	0.5	1.4264	0.3101	0.8	0.3101	0.5	0.5	0.5	0.3101
	4	0.3101	0.8	6.4343	1.49	0.5	1.4264	0.3101	0.8	0.3101	0.5	0.5	0.5	0.5
95	1	0.3101	0.8	6.4343	1.49	0.5	1.4264	0.3101	0.8	0.3101	0.5	0.5	0.5	0.3101
	2	0.3101	0.8	6.4343	1.49	0.5	1.4264	0.3101	0.8	0.3101	0.5	0.5	0.5	0.3101
	3	0.3101	0.8	6.4343	1.49	0.5	1.4264	0.3101	0.8	0.3101	0.5	0.5	0.5	0.3101
	4	0.3101	0.8	6.4343	1.49	0.5	1.4264	0.3101	0.8	0.3101	0.5	0.5	0.5	0.5
71	1	0.3101	0.8	6.4343	1.49	0.5	1.4264	0.3101	0.8	0.3101	0.5	0.5	0.5	0.3101
	2	0.3101	0.8	6.4343	1.49	0.5	1.4264	0.3101	0.8	0.3101	0.5	0.5	0.5	0.3101
	3	0.3101	0.8	6.4343	1.49	0.5	1.4264	0.3101	0.8	0.3101	0.5	0.5	0.5	0.3101
	4	0.3101	0.8	6.4343	1.49	0.5	1.4264	0.3101	0.8	0.3101	0.5	0.5	0.5	0.5
[1986]														
366a	1	0.3101	0.8	6.4343	1.49	0.5	1.4264	0.3101	0.8	0.3101	0.5	0.5	0.5	0.3101
	2	0.3101	0.8	6.4343	1.49	0.5	1.4264	0.3101	0.8	0.3101	0.5	0.5	0.5	0.3101
	3	0.3101	0.8	6.4343	1.49	0.5	1.4264	0.3101	0.8	0.3101	0.5	0.5	0.5	0.3101
	4	0.3101	0.8	6.4343	1.49	0.5	1.4264	0.3101	0.8	0.3101	0.5	0.5	0.5	0.5
368	1	0.3101	0.8	6.4343	1.49	0.5	1.4264	0.3101	0.8	0.3101	0.5	0.5	0.5	0.3101
	2	0.3101	0.8	6.4343	1.49	0.5	1.4264	0.3101	0.8	0.3101	0.5	0.5	0.5	0.3101
	3	0.3101	0.8	6.4343	1.49	0.5	1.4264	0.3101	0.8	0.3101	0.5	0.5	0.5	0.3101
	4	0.3101	0.8	6.4343	1.49	0.5	1.4264	0.3101	0.8	0.3101	0.5	0.5	0.5	0.5
368b	1	0.3101	0.8	6.4343	1.49	0.5	1.4264	0.3101	0.8	0.3101	0.5	0.5	0.5	0.3101
	2	0.3101	0.8	6.4343	1.49	0.5	1.4264	0.3101	0.8	0.3101	0.5	0.5	0.5	0.3101
	3	0.3101	0.8	6.4343	1.49	0.5	1.4264	0.3101	0.8	0.3101	0.5	0.5	0.5	0.3101
	4	0.3101	0.8	6.4343	1.49	0.5	1.4264	0.3101	0.8	0.3101	0.5	0.5	0.5	0.5
369	1	0.3101	0.8	6.4343	1.49	0.5	1.4264	0.3101	0.8	0.3101	0.5	0.5	0.5	0.3101
	2	0.3101	0.8	6.4343	1.49	0.5	1.4264	0.3101	0.8	0.3101	0.5	0.5	0.5	0.3101
	3	0.3101	0.8	6.4343	1.49	0.5	1.4264	0.3101	0.8	0.3101	0.5	0.5	0.5	0.3101
	4	0.3101	0.8	6.4343	1.49	0.5	1.4264	0.3101	0.8	0.3101	0.5	0.5	0.5	0.5
371	1	0.3101	0.8	6.4343	1.49	0.5	1.4264	0.3101	0.8	0.3101	0.5	0.5	0.5	0.3101
	2	0.3101	0.8	6.4343	1.49	0.5	1.4264	0.3101	0.8	0.3101	0.5	0.5	0.5	0.3101
	3	0.3101	0.8	6.4343	1.49	0.5	1.4264	0.3101	0.8	0.3101	0.5	0.5	0.5	0.3101
	4	0.3101	0.8	6.4343	1.49	0.5	1.4264	0.3101	0.8	0.3101	0.5	0.5	0.5	0.5
371b	1	0.3101	0.8	6.4343	1.49	0.5	1.4264	0.3101	0.8	0.3101	0.5	0.5	0.5	0.3101
	2	0.3101	0.8	6.4343	1.49	0.5	1.4264	0.3101	0.8	0.3101	0.5	0.5	0.5	0.3101
	3	0.3101	0.8	6.4343	1.49	0.5	1.4264	0.3101	0.8	0.3101	0.5	0.5	0.5	0.3101
	4	0.3101	0.8	6.4343	1.49	0.5	1.4264	0.3101	0.8	0.3101	0.5	0.5	0.5	0.5
374	1	0.3101	0.8	6.4343	1.49	0.5	1.4264	0.3101	0.8	0.3101	0.5	0.5	0.5	0.3101
	2	0.3101	0.8	6.4343	1.49	0.5	1.4264	0.3101	0.8	0.3101	0.5	0.5	0.5	0.3101
	3	0.3101	0.8	6.4343	1.49	0.5	1.4264	0.3101	0.8	0.3101	0.5	0.5	0.5	0.3101
	4	0.3101	0.8	6.4343	1.49	0.5	1.4264	0.3101	0.8	0.3101	0.5	0.5	0.5	0.5
375	1	0.3101	0.8	6.4343	1.49	0.5	1.4264	0.3101	0.8	0.3101	0.5	0.5	0.5	0.3101
	2	0.3101	0.8	6.4343	1.49	0.5	1.4264	0.3101	0.8	0.3101	0.5	0.5	0.5	0.3101
	3	0.3101	0.8	6.4343	1.49	0.5	1.4264	0.3101	0.8	0.3101	0.5	0.5	0.5	0.3101
	4	0.3101	0.8	6.4343	1.49	0.5	1.4264	0.3101	0.8	0.3101	0.5	0.5	0.5	0.5
398a	1	0.3101	0.8	6.4343	1.49	0.5	1.4264	0.3101	0.8	0.3101	0.5	0.5	0.5	0.3101
	2	0.3101	0.8	6.4343	1.49	0.5	1.4264	0.3101	0.8	0.3101	0.5	0.5	0.5	0.3101
	3	0.3101	0.8	6.4343	1.49	0.5	1.4264	0.3101	0.8	0.3101	0.5	0.5	0.5	0.3101
	4	0.3101	0.8	6.4343	1.49	0.5	1.4264	0.3101	0.8	0.3101	0.5	0.5	0.5	0.5

		N	1979	N	1979+1986	N	1986
GEO AVE (Pred/Meas)	Level 1	1	0.898602	1	0.8986024	0	
	Level 2	2	8.994113	11	1.3965432	9	0.923205
	Level 3	1	7.452305	10	1.3167636	9	1.086089
	Level 4	0		0		0	
	OVERALL	4	4.824404	22	1.3327183	18	1.00134
	S.D.(Pred/Meas)		8.717556		4.7732754		0.735685
	SD log[pred/meas]		0.514207		0.4304463		0.287956

PClip	4.183
EFACTR	1
ALFFTR	1

Calculated Model Variables:

STN NO [1979]	TROPHIC LEVEL	RESP	GROW	CONS	KU	K	ALF	NW	F	CF mg / glipid	CF*LIP mg / gtotal	STN NO [1979]	TROPHIC LEVEL	Measured "CF*LIP" (mg/g total) at trophic level:	Predicted / Measured "CF*LIP"	LOG P/M
112	1	0.1977	0.0549	2.5267	74057	4.8592	0.3101	15241	0.1594	3.58E-03	8.24E-05	112	1			
	2	0.0823	0.0229	0.3506	44316	2.9077	0.3101	14527	0.0371	3.55E-03	5.67E-05		2			
	3	0.032	0.0089	0.0511	7658.5	0.5025	0.3101	14527	0.031	3.52E-03	1.27E-04		3			
	4	0.0136	0.0038	0.0218	2059.4	0.1351	0.5	14790	0.0784	3.75E-03	3.45E-04		4			
104	1	0.1977	0.0549	2.5267	74057	4.8592	0.3101	15241	0.1594	1.47E-02	3.39E-04	104	1			
	2	0.0823	0.0229	0.3506	44316	2.9077	0.3101	14527	0.0371	1.46E-02	2.33E-04		2	1.00E-05	2.3E+01	1.3680226
	3	0.032	0.0089	0.0511	7658.5	0.5025	0.3101	14527	0.031	1.45E-02	5.22E-04		3	7.00E-05	7.5E+00	0.8722906
	4	0.0136	0.0038	0.0218	2059.4	0.1351	0.5	14790	0.0784	1.54E-02	1.42E-03		4			
95	1	0.1977	0.0549	2.5267	74057	4.8592	0.3101	15241	0.1594	1.09E-02	2.52E-04	95	1	2.80E-04	9.0E-01	-0.046432
	2	0.0823	0.0229	0.3506	44316	2.9077	0.3101	14527	0.0371	1.08E-02	1.73E-04		2	5.00E-05	3.5E+00	0.539894
	3	0.032	0.0089	0.0511	7658.5	0.5025	0.3101	14527	0.031	1.08E-02	3.87E-04		3			
	4	0.0136	0.0038	0.0218	2059.4	0.1351	0.5	14790	0.0784	1.15E-02	1.05E-03		4			
71	1	0.1977	0.0549	2.5267	74057	4.8592	0.3101	15241	0.1594	1.04E-02	2.40E-04	71	1			
	2	0.1208	0.0336	0.5145	173434	11.38	0.3101	14527	0.014	1.01E-02	6.06E-05		2			
	3	0.032	0.0089	0.0511	7658.5	0.5025	0.3101	14527	0.031	1.03E-02	3.69E-04		3			
	4	0.0136	0.0038	0.0218	2059.4	0.1351	0.5	14790	0.0784	1.09E-02	1.01E-03		4			
[1986]												[1986]				
366a	1	0.1977	0.0549	2,5267	74057	4.8592	0.3101	15241	0.1594	4.98E-03	1.14E-04	366a	1			
	2	0.1208	0.0336	0.5145	173434	11.38	0.3101	14527	0.014	4.81E-03	2.89E-05		2	5.80E-05	5.0E-01	-0.302979
	3	0.0273	0.0076	0.0436	5875.3	0.3855	0.3101	14527	0.0344	4.91E-03	1.96E-04		3	1.58E-04	1.2E+00	0.0942676
	4	0.0114	0.0032	0.0182	3520.9	0.231	0.5	14790	0.0389	5.02E-03	2.26E-04		4			
368	1	0.1977	0.0549	2.5267	74057	4.8592	0.3101	15241	0.1594	4.20E-03	9.66E-05	368	1			
	2	0.1208	0.0336	0.5145	346869	22.76	0.3101	14527	0.007	4.03E-03	1.21E-05		2	1.70E-05	7.1E-01	-0.147945
	3	0.0271	0.0075	0.0434	5846.3	0.3836	0.3101	14527	0.0344	4.14E-03	1.66E-04		3	1.24E-04	1.3E+00	0.1256279
	4	0.0114	0.0032	0.0182	3520.9	0.231	0.5	14790	0.0389	4.23E-03	1.91E-04		4			
368b	1	0.1977	0.0549	2.5267	74057	4.8592	0.3101	15241	0.1594	4.08E-03	9.39E-05	368b	1			
	2	0.1208	0.0336	0.5145	260152	17.07	0.3101	14527	0.0093	3.93E-03	1.57E-05		2	5.00E-06	3.1E+00	0.4973546
	3	0.0273	0.0076	0.0436	5875.3	0.3855	0.3101	14527	0.0344	4.03E-03	1.61E-04		3	1.70E-04	9.5E-01	-0.023534
	4	0.0114	0.0032	0.0182	3520.9	0.231	0.5	14790	0.0389	4.12E-03	1.85E-04		4			
369	1	0.1977	0.0549	2.5267	74057	4.8592	0.3101	15241	0.1594	5.06E-03	1.16E-04	369	1			
	2	0.1208	0.0336	0.5145	148658	9.7541	0.3101	14527	0.0163	4.91E-03	3.44E-05		2	1.30E-05	2.6E+00	0.4220018
	3	0.0276	0.0077	0.044	6248.3	0.41	0.3101	14527	0.0327	4.99E-03	1.89E-04		3	1.50E-04	1.3E+00	0.1013794
	4	0.0114	0.0032	0.0182	3520.9	0.231	0.5	14790	0.0389	5.11E-03	2.30E-04		4			
371	1	0.1977	0.0549	2.5267	74057	4.8592	0.3101	15241	0.1594	4.81E-03	1.11E-04	371	1			
	2	0.1208	0.0336	0.5145	173434	11.38	0.3101	14527	0.014	4.65E-03	2.79E-05		2	2.40E-05	1.2E+00	0.0654615
	3	0.0271	0.0075	0.0434	5846.3	0.3836	0.3101	14527	0.0344	4.74E-03	1.90E-04		3	1.26E-04	1.5E+00	0.177778
	4	0.0114	0.0032	0.0182	3520.9	0.231	0.5	14790	0.0389	4.85E-03	2.18E-04		4			
371b	1	0.1977	0.0549	2.5267	74057	4.8592	0.3101	15241	0.1594	4.24E-03	9.76E-05	371b	1			
	2	0.1208	0.0336	0.5145	148658	9.7541	0.3101	14527	0.0163	4.12E-03	2.88E-05		2	2.30E-05	1.3E+00	0.0977757
	3	0.0276	0.0077	0.044	6248.3	0.41	0.3101	14527	0.0327	4.18E-03	1.59E-04		3	1.63E-04	9.7E-01	-0.011158
	4	0.0114	0.0032	0.0182	3520.9	0.231	0.5	14790	0.0389	4.28E-03	1.93E-04		4			
374	1	0.1977	0.0549	2.5267	74057	4.8592	0.3101	15241	0.1594	5.02E-03	1.15E-04	374	1			
	2	0.0926	0.0257	0.3942	113900	7.4735	0.3101	14527	0.0163	4.86E-03	3.40E-05		2	1.00E-04	3.4E-01	-0.467926
	3	0.0271	0.0075	0.0434	5846.3	0.3836	0.3101	14527	0.0344	4.95E-03	1.98E-04		3	1.09E-04	1.8E+00	0.2591706
	4	0.0114	0.0032	0.0182	3520.9	0.231	0.5	14790	0.0389	5.06E-03	2.28E-04		4			
375	1	0.1977	0.0549	2.5267	74057	4.8592	0.3101	15241	0.1594	4.60E-03	1.06E-04	375	1			
	2	0.1208	0.0336	0.5145	173434	11.38	0.3101	14527	0.014	4.45E-03	2.67E-05		2	2.90E-05	9.2E-01	-0.036361
	3	0.0276	0.0077	0.044	6248.3	0.41	0.3101	14527	0.0327	4.53E-03	1.72E-04		3	1.10E-04	1.6E+00	0.194125
	4	0.0114	0.0032	0.0182	3520.9	0.231	0.5	14790	0.0389	4.64E-03	2.09E-04		4			
398a	1	0.1977	0.0549	2.5267	74057	4.8592	0.3101	15241	0.1594	1.49E-03	3.43E-05	398a	1			
	2	0.1208	0.0336	0.5145	115623	7.5865	0.3101	14527	0.0209	1.45E-03	1.31E-05		2	3.60E-05	3.6E-01	-0.439702
	3	0.0313	0.0087	0.0501	8180.5	0.5368	0.3101	14527	0.0285	1.46E-03	4.83E-05		3	1.90E-04	2.5E-01	-0.594869
	4	0.0114	0.0032	0.0182	3520.9	0.231	0.5	14790	0.0389	1.50E-03	6.77E-05		4			

THOMANN STEADY-STATE, 4 LEVEL FOOD CHAIN MODEL ASSUME: E = EFACTR * E EFACTR = 0.032 ASSUME: ALF=E*EFACTR*ALFFTR ALFFTR= 1

FOR ZINC : ESTIMATED LOG KOW = 5.66

INPUT VALUES FOR MODEL — Estimation of the Uptake Efficiency "E":

STN NO [1979]	TROPHIC LEVEL	W gm	LIP	A	ALF	BETA	GAM	DEL	FI	STN NO [1979]	TROPHIC LEVEL	Calculated from Eq. E15A	E15B	E15C	E16A	E16B	E16C	Minimum value from: E15AB	E15BC	E15ABC	E16AB	E16BC	E16ABC	E * EFACTR
112	1	0.0002	0.023	0.1	0.1	0.2	0.2	0.01	0.036	112	1	1.6982	0.8	1.1749	5.8076	0.5	0.6095	0.8	0.8	0.8	0.5	0.5	0.5	0.0256
	2	0.0024	0.006	0.3	0.3	0.2	0.2	0.01	0.036		2	1.6982	0.8	1.1749	5.8076	0.5	0.6095	0.8	0.8	0.8	0.5	0.5	0.5	0.0256
	3	1.8	0.036	0.8	0.8	0.2	0.2	0.01	0.036		3	1.6982	0.8	1.1749	5.8076	0.5	0.6095	0.8	0.8	0.8	0.5	0.5	0.5	0.0256
	4	128	0.092	0.8	0.8	0.2	0.2	0.01	0.036		4	1.6982	0.8	1.1749	5.8076	0.5	0.6095	0.8	0.8	0.8	0.5	0.5	0.5	0.016
104	1	0.0002	0.023	0.1	0.1	0.2	0.2	0.01	0.036	104	1	1.6982	0.8	1.1749	5.8076	0.5	0.6095	0.8	0.8	0.8	0.5	0.5	0.5	0.0256
	2	0.0093	0.016	0.3	0.3	0.2	0.2	0.01	0.036		2	1.6982	0.8	1.1749	5.8076	0.5	0.6095	0.8	0.8	0.8	0.5	0.5	0.5	0.0256
	3	1.8	0.036	0.8	0.8	0.2	0.2	0.01	0.036		3	1.6982	0.8	1.1749	5.8076	0.5	0.6095	0.8	0.8	0.8	0.5	0.5	0.5	0.0256
	4	128	0.092	0.8	0.8	0.2	0.2	0.01	0.036		4	1.6982	0.8	1.1749	5.8076	0.5	0.6095	0.8	0.8	0.8	0.5	0.5	0.5	0.016
95	1	0.0002	0.023	0.1	0.1	0.2	0.2	0.01	0.036	95	1	1.6982	0.8	1.1749	5.8076	0.5	0.6095	0.8	0.8	0.8	0.5	0.5	0.5	0.0256
	2	0.0093	0.016	0.3	0.3	0.2	0.2	0.01	0.036		2	1.6982	0.8	1.1749	5.8076	0.5	0.6095	0.8	0.8	0.8	0.5	0.5	0.5	0.0256
	3	1.8	0.036	0.8	0.8	0.2	0.2	0.01	0.036		3	1.6982	0.8	1.1749	5.8076	0.5	0.6095	0.8	0.8	0.8	0.5	0.5	0.5	0.0256
	4	128	0.092	0.8	0.8	0.2	0.2	0.01	0.036		4	1.6982	0.8	1.1749	5.8076	0.5	0.6095	0.8	0.8	0.8	0.5	0.5	0.5	0.016
71	1	0.0002	0.023	0.1	0.1	0.2	0.2	0.01	0.036	71	1	1.6982	0.8	1.1749	5.8076	0.5	0.6095	0.8	0.8	0.8	0.5	0.5	0.5	0.0256
	2	0.0093	0.016	0.3	0.3	0.2	0.2	0.01	0.036		2	1.6982	0.8	1.1749	5.8076	0.5	0.6095	0.8	0.8	0.8	0.5	0.5	0.5	0.0256
	3	1.8	0.036	0.8	0.8	0.2	0.2	0.01	0.036		3	1.6982	0.8	1.1749	5.8076	0.5	0.6095	0.8	0.8	0.8	0.5	0.5	0.5	0.0256
	4	128	0.092	0.8	0.8	0.2	0.2	0.01	0.036		4	1.6982	0.8	1.1749	5.8076	0.5	0.6095	0.8	0.8	0.8	0.5	0.5	0.5	0.016
[1986]										[1986]														
366a	1	0.0002	0.023	0.1	0.1	0.2	0.2	0.01	0.036	366a	1	1.6982	0.8	1.1749	5.8076	0.5	0.6095	0.8	0.8	0.8	0.5	0.5	0.5	0.0256
	2	0.0024	0.006	0.3	0.3	0.2	0.2	0.01	0.036		2	1.6982	0.8	1.1749	5.8076	0.5	0.6095	0.8	0.8	0.8	0.5	0.5	0.5	0.0256
	3	4	0.04	0.8	0.8	0.2	0.2	0.01	0.036		3	1.6982	0.8	1.1749	5.8076	0.5	0.6095	0.8	0.8	0.8	0.5	0.5	0.5	0.0256
	4	313	0.045	0.8	0.8	0.2	0.2	0.01	0.036		4	1.6982	0.8	1.1749	5.8076	0.5	0.6095	0.8	0.8	0.8	0.5	0.5	0.5	0.016
368	1	0.0002	0.023	0.1	0.1	0.2	0.2	0.01	0.036	368	1	1.6982	0.8	1.1749	5.8076	0.5	0.6095	0.8	0.8	0.8	0.5	0.5	0.5	0.0256
	2	0.0024	0.003	0.3	0.3	0.2	0.2	0.01	0.036		2	1.6982	0.8	1.1749	5.8076	0.5	0.6095	0.8	0.8	0.8	0.5	0.5	0.5	0.0256
	3	4.1	0.04	0.8	0.8	0.2	0.2	0.01	0.036		3	1.6982	0.8	1.1749	5.8076	0.5	0.6095	0.8	0.8	0.8	0.5	0.5	0.5	0.0256
	4	313	0.045	0.8	0.8	0.2	0.2	0.01	0.036		4	1.6982	0.8	1.1749	5.8076	0.5	0.6095	0.8	0.8	0.8	0.5	0.5	0.5	0.016
368b	1	0.0002	0.023	0.1	0.1	0.2	0.2	0.01	0.036	368b	1	1.6982	0.8	1.1749	5.8076	0.5	0.6095	0.8	0.8	0.8	0.5	0.5	0.5	0.0256
	2	0.0024	0.004	0.3	0.3	0.2	0.2	0.01	0.036		2	1.6982	0.8	1.1749	5.8076	0.5	0.6095	0.8	0.8	0.8	0.5	0.5	0.5	0.0256
	3	4	0.04	0.8	0.8	0.2	0.2	0.01	0.036		3	1.6982	0.8	1.1749	5.8076	0.5	0.6095	0.8	0.8	0.8	0.5	0.5	0.5	0.0256
	4	313	0.045	0.8	0.8	0.2	0.2	0.01	0.036		4	1.6982	0.8	1.1749	5.8076	0.5	0.6095	0.8	0.8	0.8	0.5	0.5	0.5	0.016
369	1	0.0002	0.023	0.1	0.1	0.2	0.2	0.01	0.036	369	1	1.6982	0.8	1.1749	5.8076	0.5	0.6095	0.8	0.8	0.8	0.5	0.5	0.5	0.0256
	2	0.0024	0.007	0.3	0.3	0.2	0.2	0.01	0.036		2	1.6982	0.8	1.1749	5.8076	0.5	0.6095	0.8	0.8	0.8	0.5	0.5	0.5	0.0256
	3	3.8	0.038	0.8	0.8	0.2	0.2	0.01	0.036		3	1.6982	0.8	1.1749	5.8076	0.5	0.6095	0.8	0.8	0.8	0.5	0.5	0.5	0.0256
	4	313	0.045	0.8	0.8	0.2	0.2	0.01	0.036		4	1.6982	0.8	1.1749	5.8076	0.5	0.6095	0.8	0.8	0.8	0.5	0.5	0.5	0.016
371	1	0.0002	0.023	0.1	0.1	0.2	0.2	0.01	0.036	371	1	1.6982	0.8	1.1749	5.8076	0.5	0.6095	0.8	0.8	0.8	0.5	0.5	0.5	0.0256
	2	0.0024	0.006	0.3	0.3	0.2	0.2	0.01	0.036		2	1.6982	0.8	1.1749	5.8076	0.5	0.6095	0.8	0.8	0.8	0.5	0.5	0.5	0.0256
	3	4.1	0.04	0.8	0.8	0.2	0.2	0.01	0.036		3	1.6982	0.8	1.1749	5.8076	0.5	0.6095	0.8	0.8	0.8	0.5	0.5	0.5	0.0256
	4	313	0.045	0.8	0.8	0.2	0.2	0.01	0.036		4	1.6982	0.8	1.1749	5.8076	0.5	0.6095	0.8	0.8	0.8	0.5	0.5	0.5	0.016
371b	1	0.0002	0.023	0.1	0.1	0.2	0.2	0.01	0.036	371b	1	1.6982	0.8	1.1749	5.8076	0.5	0.6095	0.8	0.8	0.8	0.5	0.5	0.5	0.0256
	2	0.0024	0.007	0.3	0.3	0.2	0.2	0.01	0.036		2	1.6982	0.8	1.1749	5.8076	0.5	0.6095	0.8	0.8	0.8	0.5	0.5	0.5	0.0256
	3	3.8	0.038	0.8	0.8	0.2	0.2	0.01	0.036		3	1.6982	0.8	1.1749	5.8076	0.5	0.6095	0.8	0.8	0.8	0.5	0.5	0.5	0.0256
	4	313	0.045	0.8	0.8	0.2	0.2	0.01	0.036		4	1.6982	0.8	1.1749	5.8076	0.5	0.6095	0.8	0.8	0.8	0.5	0.5	0.5	0.016
374	1	0.0002	0.023	0.1	0.1	0.2	0.2	0.01	0.036	374	1	1.6982	0.8	1.1749	5.8076	0.5	0.6095	0.8	0.8	0.8	0.5	0.5	0.5	0.0256
	2	0.0089	0.007	0.3	0.3	0.2	0.2	0.01	0.036		2	1.6982	0.8	1.1749	5.8076	0.5	0.6095	0.8	0.8	0.8	0.5	0.5	0.5	0.0256
	3	4.1	0.04	0.8	0.8	0.2	0.2	0.01	0.036		3	1.6982	0.8	1.1749	5.8076	0.5	0.6095	0.8	0.8	0.8	0.5	0.5	0.5	0.0256
	4	313	0.045	0.8	0.8	0.2	0.2	0.01	0.036		4	1.6982	0.8	1.1749	5.8076	0.5	0.6095	0.8	0.8	0.8	0.5	0.5	0.5	0.016
375	1	0.0002	0.023	0.1	0.1	0.2	0.2	0.01	0.036	375	1	1.6982	0.8	1.1749	5.8076	0.5	0.6095	0.8	0.8	0.8	0.5	0.5	0.5	0.0256
	2	0.0024	0.006	0.3	0.3	0.2	0.2	0.01	0.036		2	1.6982	0.8	1.1749	5.8076	0.5	0.6095	0.8	0.8	0.8	0.5	0.5	0.5	0.0256
	3	3.8	0.038	0.8	0.8	0.2	0.2	0.01	0.036		3	1.6982	0.8	1.1749	5.8076	0.5	0.6095	0.8	0.8	0.8	0.5	0.5	0.5	0.0256
	4	313	0.045	0.8	0.8	0.2	0.2	0.01	0.036		4	1.6982	0.8	1.1749	5.8076	0.5	0.6095	0.8	0.8	0.8	0.5	0.5	0.5	0.016
398a	1	0.0002	0.023	0.1	0.1	0.2	0.2	0.01	0.036	398a	1	1.6982	0.8	1.1749	5.8076	0.5	0.6095	0.8	0.8	0.8	0.5	0.5	0.5	0.0256
	2	0.0024	0.009	0.3	0.3	0.2	0.2	0.01	0.036		2	1.6982	0.8	1.1749	5.8076	0.5	0.6095	0.8	0.8	0.8	0.5	0.5	0.5	0.0256
	3	2	0.033	0.8	0.8	0.2	0.2	0.01	0.036		3	1.6982	0.8	1.1749	5.8076	0.5	0.6095	0.8	0.8	0.8	0.5	0.5	0.5	0.0256
	4	313	0.045	0.8	0.8	0.2	0.2	0.01	0.036		4	1.6982	0.8	1.1749	5.8076	0.5	0.6095	0.8	0.8	0.8	0.5	0.5	0.5	0.016

	N	1979	N	1979+1986	N	1986
GEO AVE (Pred/Meas) Level 1	2	0.868747	2	0.8687472	0	
Level 2	4	0.450418	13	0.7830158	9	1.001166
Level 3	0		9	1.0027692	9	1.002769
Level 4	0		0		0	
OVERALL	6	0.560671	24	0.866597	18	1.001967
S.D. (Pred/Meas)		0.40854		1.0414589		1.15034
SD log[pred/meas]		0.519807		0.3934588		0.316942

PClip	5.66
EFACTR	0.032
ALFFTR	1

Calculated Model Variables:

STN NO [1979]	TROPHIC LEVEL	RESP	GROW	CONS	KU	K	ALF	NW	F	CF mg / glipid	CF*LIP mg / gtotal	STN NO [1979]	TROPHIC LEVEL	Measured "CF*LIP" (mg/g total) at trophic level:	Predicted / Measured "CF*LIP"	LOG P/M
112	1	0.1977	0.0549	2.5267	6113.7	0.0134	0.0256	457088	0.947	2.07E+00	4.76E-02	112	1	0.081	5.9E-01	-0.230863
	2	0.1208	0.0336	0.5145	14318	0.0313	0.0256	24242	0.203	5.30E-01	3.18E-03		2	0.078	4.1E-02	-1.389709
	3	0.032	0.0089	0.0511	632.24	0.0014	0.0256	24242	0.1274	1.77E-01	6.38E-03		3			
	4	0.0136	0.0038	0.0218	65.901	0.0001	0.016	15459	0.0886	8.57E-02	7.89E-03		4			
104	1	0.1977	0.0549	2.5267	6113.7	0.0134	0.0256	457088	0.947	6.50E+00	1.50E-01	104	1			
	2	0.0918	0.0255	0.3909	4078.7	0.0089	0.0256	24242	0.2908	2.24E+00	3.58E-02		2	3.20E-02	1.1E+00	0.0484695
	3	0.032	0.0089	0.0511	632.24	0.0014	0.0256	24242	0.1274	6.30E-01	2.27E-02		3			
	4	0.0136	0.0038	0.0218	65.901	0.0001	0.016	15459	0.0886	2.76E-01	2.54E-02		4			
95	1	0.1977	0.0549	2.5267	6113.7	0.0134	0.0256	457088	0.947	2.51E+01	5.78E-01	95	1	4.50E-01	1.3E+00	0.10865
	2	0.0918	0.0255	0.3909	4078.7	0.0089	0.0256	24242	0.2908	8.64E+00	1.38E-01		2	1.50E-01	9.2E-01	-0.03554
	3	0.032	0.0089	0.0511	632.24	0.0014	0.0256	24242	0.1274	2.43E+00	8.76E-02		3			
	4	0.0136	0.0038	0.0218	65.901	0.0001	0.016	15459	0.0886	1.07E+00	9.80E-02		4			
71	1	0.1977	0.0549	2.5267	6113.7	0.0134	0.0256	457088	0.947	8.73E+00	2.01E-01	71	1			
	2	0.0918	0.0255	0.3909	4078.7	0.0089	0.0256	24242	0.2908	3.00E+00	4.80E-02		2	0.049	9.8E-01	-0.008759
	3	0.032	0.0089	0.0511	632.24	0.0014	0.0256	24242	0.1274	8.45E-01	3.04E-02		3			
	4	0.0136	0.0038	0.0218	65.901	0.0001	0.016	15459	0.0886	3.70E-01	3.41E-02		4			
[1986]												[1986]				
366a	1	0.1977	0.0549	2.5267	6113.7	0.0134	0.0256	457088	0.947	7.40E+00	1.70E-01	366a	1			
	2	0.1208	0.0336	0.5145	14318	0.0313	0.0256	24242	0.203	1.89E+00	1.14E-02		2	1.00E-02	1.1E+00	0.0555576
	3	0.0273	0.0076	0.0436	485.03	0.0011	0.0256	24242	0.1291	6.37E-01	2.55E-02		3	3.30E-02	7.7E-01	-0.11239
	4	0.0114	0.0032	0.0182	112.67	0.0002	0.016	15459	0.0854	3.05E-01	1.37E-02		4			
368	1	0.1977	0.0549	2.5267	6113.7	0.0134	0.0256	457088	0.947	2.26E+01	5.20E-01	368	1			
	2	0.1208	0.0336	0.5145	28636	0.0626	0.0256	24242	0.1369	4.29E+00	1.29E-02		2	2.30E-02	5.6E-01	-0.251884
	3	0.0271	0.0075	0.0434	482.64	0.0011	0.0256	24242	0.1291	1.75E+00	7.01E-02		3	4.30E-02	1.6E+00	0.2123193
	4	0.0114	0.0032	0.0182	112.67	0.0002	0.016	15459	0.0854	9.14E-01	4.11E-02		4			
368b	1	0.1977	0.0549	2.5267	6113.7	0.0134	0.0256	457088	0.947	6.78E+00	1.56E-01	368b	1			
	2	0.1208	0.0336	0.5145	21477	0.047	0.0256	24242	0.1635	1.47E+00	5.87E-03		2	1.30E-02	4.5E-01	-0.345224
	3	0.0273	0.0076	0.0436	485.03	0.0011	0.0256	24242	0.1291	5.49E-01	2.20E-02		3	2.70E-02	8.1E-01	-0.089771
	4	0.0114	0.0032	0.0182	112.67	0.0002	0.016	15459	0.0854	2.76E-01	1.24E-02		4			
369	1	0.1977	0.0549	2.5267	6113.7	0.0134	0.0256	457088	0.947	3.44E+01	7.92E-01	369	1			
	2	0.1208	0.0336	0.5145	12272	0.0268	0.0256	24242	0.2181	9.34E+00	6.54E-02		2	1.60E-02	4.1E+00	0.6111813
	3	0.0276	0.0077	0.044	515.82	0.0011	0.0256	24242	0.1283	3.02E+00	1.15E-01		3	3.10E-02	3.7E+00	0.5690712
	4	0.0114	0.0032	0.0182	112.67	0.0002	0.016	15459	0.0854	1.42E+00	6.40E-02		4			
371	1	0.1977	0.0549	2.5267	6113.7	0.0134	0.0256	457088	0.947	9.01E+00	2.07E-01	371	1			
	2	0.1208	0.0336	0.5145	14318	0.0313	0.0256	24242	0.203	2.31E+00	1.38E-02		2	1.40E-02	9.9E-01	-0.004855
	3	0.0271	0.0075	0.0434	482.64	0.0011	0.0256	24242	0.1291	7.76E-01	3.10E-02		3	3.80E-02	8.2E-01	-0.087945
	4	0.0114	0.0032	0.0182	112.67	0.0002	0.016	15459	0.0854	3.71E-01	1.67E-02		4			
371b	1	0.1977	0.0549	2.5267	6113.7	0.0134	0.0256	457088	0.947	1.87E+01	4.31E-01	371b	1			
	2	0.1208	0.0336	0.5145	12272	0.0268	0.0256	24242	0.2181	5.08E+00	3.56E-02		2	1.00E-02	3.6E+00	0.5510399
	3	0.0276	0.0077	0.044	515.82	0.0011	0.0256	24242	0.1283	1.65E+00	6.25E-02		3	4.20E-02	1.5E+00	0.1729223
	4	0.0114	0.0032	0.0182	112.67	0.0002	0.016	15459	0.0854	7.74E-01	3.48E-02		4			
374	1	0.1977	0.0549	2.5267	6113.7	0.0134	0.0256	457088	0.947	9.99E+00	2.30E-01	374	1			
	2	0.0926	0.0257	0.3942	9402.9	0.0206	0.0256	24242	0.2181	2.71E+00	1.90E-02		2	3.50E-02	5.4E-01	-0.266257
	3	0.0271	0.0075	0.0434	482.64	0.0011	0.0256	24242	0.1291	8.80E-01	3.52E-02		3	2.60E-02	1.4E+00	0.1313563
	4	0.0114	0.0032	0.0182	112.67	0.0002	0.016	15459	0.0854	4.13E-01	1.86E-02		4			
375	1	0.1977	0.0549	2.5267	6113.7	0.0134	0.0256	457088	0.947	8.40E+00	1.93E-01	375	1			
	2	0.1208	0.0336	0.5145	14318	0.0313	0.0256	24242	0.203	2.15E+00	1.29E-02		2	1.60E-02	8.1E-01	-0.093587
	3	0.0276	0.0077	0.044	515.82	0.0011	0.0256	24242	0.1283	7.21E-01	2.74E-02		3	4.70E-02	5.8E-01	-0.234348
	4	0.0114	0.0032	0.0182	112.67	0.0002	0.016	15459	0.0854	3.45E-01	1.55E-02		4			
398a	1	0.1977	0.0549	2.5267	6113.7	0.0134	0.0256	457088	0.947	2.74E+00	6.31E-02	398a	1			
	2	0.1208	0.0336	0.5145	9545.2	0.0209	0.0256	24242	0.242	6.10E-01	7.29E-03		2	1.30E-02	5.6E-01	-0.251416
	3	0.0313	0.0087	0.0501	675.34	0.0015	0.0256	24242	0.1258	2.47E-01	8.17E-03		3	2.90E-02	2.8E-01	-0.550406
	4	0.0114	0.0032	0.0182	112.67	0.0002	0.016	15459	0.0854	1.14E-01	5.13E-03		4			

THOMANN STEADY-STATE, 4 LEVEL FOOD CHAIN MODEL ASSUME: E = EFACTR * E ASSUME: ALF=E*EFACTR*ALFFTR

FOR PCBs : ESTIMATED LOG KOW = 6.081 EFACTR = 1 ALFFTR = 1

INPUT VALUES FOR MODEL

STN NO	TROPHIC LEVEL	W (gm)	LIP	A	ALF	BETA	GAM	DEL	FI
[1979]									
112	1	0.0002	0.023	0.1	0.1	0.2	0.2	0.01	0.036
	2	0.0024	0.006	0.3	0.3	0.2	0.2	0.01	0.036
	3	1.8	0.036	0.8	0.8	0.2	0.2	0.01	0.036
	4	128	0.092	0.8	0.8	0.2	0.2	0.01	0.036
104	1	0.0002	0.023	0.1	0.1	0.2	0.2	0.01	0.036
	2	0.0093	0.016	0.3	0.3	0.2	0.2	0.01	0.036
	3	1.8	0.036	0.8	0.8	0.2	0.2	0.01	0.036
	4	128	0.092	0.8	0.8	0.2	0.2	0.01	0.036
95	1	0.0002	0.023	0.1	0.1	0.2	0.2	0.01	0.036
	2	0.0093	0.016	0.3	0.3	0.2	0.2	0.01	0.036
	3	1.8	0.036	0.8	0.8	0.2	0.2	0.01	0.036
	4	128	0.092	0.8	0.8	0.2	0.2	0.01	0.036
71	1	0.0002	0.023	0.1	0.1	0.2	0.2	0.01	0.036
	2	0.0093	0.016	0.3	0.3	0.2	0.2	0.01	0.036
	3	1.8	0.036	0.8	0.8	0.2	0.2	0.01	0.036
	4	128	0.092	0.8	0.8	0.2	0.2	0.01	0.036
[1986]									
366a	1	0.0002	0.023	0.1	0.1	0.2	0.2	0.01	0.036
	2	0.0024	0.006	0.3	0.3	0.2	0.2	0.01	0.036
	3	2.9	0.025	0.8	0.8	0.2	0.2	0.01	0.036
	4	313	0.045	0.8	0.8	0.2	0.2	0.01	0.036
368	1	0.0002	0.023	0.1	0.1	0.2	0.2	0.01	0.036
	2	0.0024	0.003	0.3	0.3	0.2	0.2	0.01	0.036
	3	4.1	0.012	0.8	0.8	0.2	0.2	0.01	0.036
	4	313	0.045	0.8	0.8	0.2	0.2	0.01	0.036
368b	1	0.0002	0.023	0.1	0.1	0.2	0.2	0.01	0.036
	2	0.0024	0.004	0.3	0.3	0.2	0.2	0.01	0.036
	3	4	0.049	0.8	0.8	0.2	0.2	0.01	0.036
	4	313	0.045	0.8	0.8	0.2	0.2	0.01	0.036
369	1	0.0002	0.023	0.1	0.1	0.2	0.2	0.01	0.036
	2	0.0024	0.007	0.3	0.3	0.2	0.2	0.01	0.036
	3	3.8	0.036	0.8	0.8	0.2	0.2	0.01	0.036
	4	313	0.045	0.8	0.8	0.2	0.2	0.01	0.036
371	1	0.0002	0.023	0.1	0.1	0.2	0.2	0.01	0.036
	2	0.0024	0.006	0.3	0.3	0.2	0.2	0.01	0.036
	3	4.1	0.022	0.8	0.8	0.2	0.2	0.01	0.036
	4	313	0.045	0.8	0.8	0.2	0.2	0.01	0.036
371b	1	0.0002	0.023	0.1	0.1	0.2	0.2	0.01	0.036
	2	0.0024	0.007	0.3	0.3	0.2	0.2	0.01	0.036
	3	3.8	0.032	0.8	0.8	0.2	0.2	0.01	0.036
	4	313	0.045	0.8	0.8	0.2	0.2	0.01	0.036
374	1	0.0002	0.023	0.1	0.1	0.2	0.2	0.01	0.036
	2	0.0089	0.007	0.3	0.3	0.2	0.2	0.01	0.036
	3	4.1	0.0086	0.8	0.8	0.2	0.2	0.01	0.036
	4	313	0.045	0.8	0.8	0.2	0.2	0.01	0.036
375	1	0.0002	0.023	0.1	0.1	0.2	0.2	0.01	0.036
	2	0.0024	0.006	0.3	0.3	0.2	0.2	0.01	0.036
	3	3.8	0.02	0.8	0.8	0.2	0.2	0.01	0.036
	4	313	0.045	0.8	0.8	0.2	0.2	0.01	0.036
398a	1	0.0002	0.023	0.1	0.1	0.2	0.2	0.01	0.036
	2	0.0024	0.009	0.3	0.3	0.2	0.2	0.01	0.036
	3	2	0.03	0.8	0.8	0.2	0.2	0.01	0.036
	4	313	0.045	0.8	0.8	0.2	0.2	0.01	0.036

Estimation of the Uptake Efficiency "E":

STN NO	TROPHIC LEVEL	Calculated from Eq. E15A	E15B	E15C	E16A	E16B	E16C	Minimum value from: E15AB	E15BC	E15ABC	E16AB	E16BC	E16ABC	E * EFACTR
[1979]														
112	1	2.7574	0.8	0.7236	8.5585	0.5	0.4784	0.8	0.7236	0.7236	0.5	0.4784	0.4784	0.7236
	2	2.7574	0.8	0.7236	8.5585	0.5	0.4784	0.8	0.7236	0.7236	0.5	0.4784	0.4784	0.7236
	3	2.7574	0.8	0.7236	8.5585	0.5	0.4784	0.8	0.7236	0.7236	0.5	0.4784	0.4784	0.7236
	4	2.7574	0.8	0.7236	8.5585	0.5	0.4784	0.8	0.7236	0.7236	0.5	0.4784	0.4784	0.4784
104	1	2.7574	0.8	0.7236	8.5585	0.5	0.4784	0.8	0.7236	0.7236	0.5	0.4784	0.4784	0.7236
	2	2.7574	0.8	0.7236	8.5585	0.5	0.4784	0.8	0.7236	0.7236	0.5	0.4784	0.4784	0.7236
	3	2.7574	0.8	0.7236	8.5585	0.5	0.4784	0.8	0.7236	0.7236	0.5	0.4784	0.4784	0.7236
	4	2.7574	0.8	0.7236	8.5585	0.5	0.4784	0.8	0.7236	0.7236	0.5	0.4784	0.4784	0.4784
95	1	2.7574	0.8	0.7236	8.5585	0.5	0.4784	0.8	0.7236	0.7236	0.5	0.4784	0.4784	0.7236
	2	2.7574	0.8	0.7236	8.5585	0.5	0.4784	0.8	0.7236	0.7236	0.5	0.4784	0.4784	0.7236
	3	2.7574	0.8	0.7236	8.5585	0.5	0.4784	0.8	0.7236	0.7236	0.5	0.4784	0.4784	0.7236
	4	2.7574	0.8	0.7236	8.5585	0.5	0.4784	0.8	0.7236	0.7236	0.5	0.4784	0.4784	0.4784
71	1	2.7574	0.8	0.7236	8.5585	0.5	0.4784	0.8	0.7236	0.7236	0.5	0.4784	0.4784	0.7236
	2	2.7574	0.8	0.7236	8.5585	0.5	0.4784	0.8	0.7236	0.7236	0.5	0.4784	0.4784	0.7236
	3	2.7574	0.8	0.7236	8.5585	0.5	0.4784	0.8	0.7236	0.7236	0.5	0.4784	0.4784	0.7236
	4	2.7574	0.8	0.7236	8.5585	0.5	0.4784	0.8	0.7236	0.7236	0.5	0.4784	0.4784	0.4784
[1986]														
366a	1	2.7574	0.8	0.7236	8.5585	0.5	0.4784	0.8	0.7236	0.7236	0.5	0.4784	0.4784	0.7236
	2	2.7574	0.8	0.7236	8.5585	0.5	0.4784	0.8	0.7236	0.7236	0.5	0.4784	0.4784	0.7236
	3	2.7574	0.8	0.7236	8.5585	0.5	0.4784	0.8	0.7236	0.7236	0.5	0.4784	0.4784	0.7236
	4	2.7574	0.8	0.7236	8.5585	0.5	0.4784	0.8	0.7236	0.7236	0.5	0.4784	0.4784	0.4784
368	1	2.7574	0.8	0.7236	8.5585	0.5	0.4784	0.8	0.7236	0.7236	0.5	0.4784	0.4784	0.7236
	2	2.7574	0.8	0.7236	8.5585	0.5	0.4784	0.8	0.7236	0.7236	0.5	0.4784	0.4784	0.7236
	3	2.7574	0.8	0.7236	8.5585	0.5	0.4784	0.8	0.7236	0.7236	0.5	0.4784	0.4784	0.7236
	4	2.7574	0.8	0.7236	8.5585	0.5	0.4784	0.8	0.7236	0.7236	0.5	0.4784	0.4784	0.4784
368b	1	2.7574	0.8	0.7236	8.5585	0.5	0.4784	0.8	0.7236	0.7236	0.5	0.4784	0.4784	0.7236
	2	2.7574	0.8	0.7236	8.5585	0.5	0.4784	0.8	0.7236	0.7236	0.5	0.4784	0.4784	0.7236
	3	2.7574	0.8	0.7236	8.5585	0.5	0.4784	0.8	0.7236	0.7236	0.5	0.4784	0.4784	0.7236
	4	2.7574	0.8	0.7236	8.5585	0.5	0.4784	0.8	0.7236	0.7236	0.5	0.4784	0.4784	0.4784
369	1	2.7574	0.8	0.7236	8.5585	0.5	0.4784	0.8	0.7236	0.7236	0.5	0.4784	0.4784	0.7236
	2	2.7574	0.8	0.7236	8.5585	0.5	0.4784	0.8	0.7236	0.7236	0.5	0.4784	0.4784	0.7236
	3	2.7574	0.8	0.7236	8.5585	0.5	0.4784	0.8	0.7236	0.7236	0.5	0.4784	0.4784	0.7236
	4	2.7574	0.8	0.7236	8.5585	0.5	0.4784	0.8	0.7236	0.7236	0.5	0.4784	0.4784	0.4784
371	1	2.7574	0.8	0.7236	8.5585	0.5	0.4784	0.8	0.7236	0.7236	0.5	0.4784	0.4784	0.7236
	2	2.7574	0.8	0.7236	8.5585	0.5	0.4784	0.8	0.7236	0.7236	0.5	0.4784	0.4784	0.7236
	3	2.7574	0.8	0.7236	8.5585	0.5	0.4784	0.8	0.7236	0.7236	0.5	0.4784	0.4784	0.7236
	4	2.7574	0.8	0.7236	8.5585	0.5	0.4784	0.8	0.7236	0.7236	0.5	0.4784	0.4784	0.4784
371b	1	2.7574	0.8	0.7236	8.5585	0.5	0.4784	0.8	0.7236	0.7236	0.5	0.4784	0.4784	0.7236
	2	2.7574	0.8	0.7236	8.5585	0.5	0.4784	0.8	0.7236	0.7236	0.5	0.4784	0.4784	0.7236
	3	2.7574	0.8	0.7236	8.5585	0.5	0.4784	0.8	0.7236	0.7236	0.5	0.4784	0.4784	0.7236
	4	2.7574	0.8	0.7236	8.5585	0.5	0.4784	0.8	0.7236	0.7236	0.5	0.4784	0.4784	0.4784
374	1	2.7574	0.8	0.7236	8.5585	0.5	0.4784	0.8	0.7236	0.7236	0.5	0.4784	0.4784	0.7236
	2	2.7574	0.8	0.7236	8.5585	0.5	0.4784	0.8	0.7236	0.7236	0.5	0.4784	0.4784	0.7236
	3	2.7574	0.8	0.7236	8.5585	0.5	0.4784	0.8	0.7236	0.7236	0.5	0.4784	0.4784	0.7236
	4	2.7574	0.8	0.7236	8.5585	0.5	0.4784	0.8	0.7236	0.7236	0.5	0.4784	0.4784	0.4784
375	1	2.7574	0.8	0.7236	8.5585	0.5	0.4784	0.8	0.7236	0.7236	0.5	0.4784	0.4784	0.7236
	2	2.7574	0.8	0.7236	8.5585	0.5	0.4784	0.8	0.7236	0.7236	0.5	0.4784	0.4784	0.7236
	3	2.7574	0.8	0.7236	8.5585	0.5	0.4784	0.8	0.7236	0.7236	0.5	0.4784	0.4784	0.7236
	4	2.7574	0.8	0.7236	8.5585	0.5	0.4784	0.8	0.7236	0.7236	0.5	0.4784	0.4784	0.4784
398a	1	2.7574	0.8	0.7236	8.5585	0.5	0.4784	0.8	0.7236	0.7236	0.5	0.4784	0.4784	0.7236
	2	2.7574	0.8	0.7236	8.5585	0.5	0.4784	0.8	0.7236	0.7236	0.5	0.4784	0.4784	0.7236
	3	2.7574	0.8	0.7236	8.5585	0.5	0.4784	0.8	0.7236	0.7236	0.5	0.4784	0.4784	0.7236
	4	2.7574	0.8	0.7236	8.5585	0.5	0.4784	0.8	0.7236	0.7236	0.5	0.4784	0.4784	0.4784

	N	1979	N	1979+1986	N	1986
GEO AVE (Pred/Meas) Level 1	2	2.310136	2	2.3101364	0	
Level 2	4	5.563282	13	1.696454	9	1.000697
Level 3	1	137.9377	1	137.93767	0	
Level 4	1	57.53931	1	57.539311	0	
OVERALL	8	8.93369	17	2.8035229	9	1.000697
S.D. (Pred/Meas)		44.15915		33.984659		0.631151
SD log[pred/meas]		0.831374		0.7822923		0.340914

PClip	6.081
EFACTR	1
ALFFTR	1

Calculated Model Variables:

STN NO	TROPHIC LEVEL	RESP	GROW	CONS	KU	K	ALF	NW	F	CF mg / glipid	CF*LIP mg / gtotal	STN NO	TROPHIC LEVEL	Measured "CF*LIP" (mg/g total) at trophic level:	Predicted / Measured "CF*LIP"	LOG P/M
[1979]												[1979]				
112	1	0.1977	0.0549	2.5267	172809	0.1434	0.7236	1E+06	9.2184	8.84E-04	2.03E-05	112	1	0.00002	1.0E+00	0.0072582
	2	0.1208	0.0336	0.5145	404702	0.3358	0.7236	452115	1.0079	1.22E-03	7.34E-06		2	0.000024	3.1E-01	-0.514643
	3	0.032	0.0089	0.0511	17871	0.0148	0.7236	452115	1.5595	2.24E-03	8.06E-05		3			
	4	0.0136	0.0038	0.0218	1970.2	0.0016	0.4784	342425	1.9215	4.55E-03	4.19E-04		4			
104	1	0.1977	0.0549	2.5267	172809	0.1434	0.7236	1E+06	9.2184	1.67E-02	3.83E-04	104	1			
	2	0.0918	0.0255	0.3909	115286	0.0957	0.7236	452115	2.3344	4.51E-02	7.22E-04		2	2.00E-05	3.6E+01	1.5575745
	3	0.032	0.0089	0.0511	17871	0.0148	0.7236	452115	1.5595	7.66E-02	2.76E-03		3	2.00E-05	1.4E+02	2.1396829
	4	0.0136	0.0038	0.0218	1970.2	0.0016	0.4784	342425	1.9215	1.52E-01	1.40E-02		4	0.000243	5.8E+01	1.7599647
95	1	0.1977	0.0549	2.5267	172809	0.1434	0.7236	1E+06	9.2184	4.56E-03	1.05E-04	95	1	2.00E-05	5.2E+00	0.720017
	2	0.0918	0.0255	0.3909	115286	0.0957	0.7236	452115	2.3344	1.24E-02	1.98E-04		2	2.00E-05	9.9E+00	0.9953059
	3	0.032	0.0089	0.0511	17871	0.0148	0.7236	452115	1.5595	2.10E-02	7.56E-04		3			
	4	0.0136	0.0038	0.0218	1970.2	0.0016	0.4784	342425	1.9215	4.16E-02	3.83E-03		4			
71	1	0.1977	0.0549	2.5267	172809	0.1434	0.7236	1E+06	9.2184	4.05E-03	9.31E-05	71	1			
	2	0.0918	0.0255	0.3909	115286	0.0957	0.7236	452115	2.3344	1.10E-02	1.75E-04		2	0.00002	8.8E+00	0.9430868
	3	0.032	0.0089	0.0511	17871	0.0148	0.7236	452115	1.5595	1.86E-02	6.70E-04		3			
	4	0.0136	0.0038	0.0218	1970.2	0.0016	0.4784	342425	1.9215	3.69E-02	3.40E-03		4			
[1986]												[1986]				
366a	1	0.1977	0.0549	2.5267	172809	0.1434	0.7236	1E+06	9.2184	1.75E-02	4.04E-04	366a	1			
	2	0.1208	0.0336	0.5145	404702	0.3358	0.7236	452115	1.0079	2.43E-02	1.46E-04		2	8.50E-05	1.7E+00	0.2337255
	3	0.0291	0.0081	0.0465	23393	0.0194	0.7236	452115	1.223	3.63E-02	9.07E-04		3			
	4	0.0114	0.0032	0.0182	3368.4	0.0028	0.4784	342425	1.4614	5.80E-02	2.61E-03		4			
368	1	0.1977	0.0549	2.5267	172809	0.1434	0.7236	1E+06	9.2184	7.21E-03	1.66E-04	368	1			
	2	0.1208	0.0336	0.5145	809404	0.6717	0.7236	452115	0.5279	6.51E-03	1.95E-05		2	8.00E-05	2.4E-01	-0.612573
	3	0.0271	0.0075	0.0434	45474	0.0377	0.7236	452115	0.693	7.21E-03	8.66E-05		3			
	4	0.0114	0.0032	0.0182	3368.4	0.0028	0.4784	342425	1.4614	1.26E-02	5.66E-04		4			
368b	1	0.1977	0.0549	2.5267	172809	0.1434	0.7236	1E+06	9.2184	6.30E-03	1.45E-04	368b	1			
	2	0.1208	0.0336	0.5145	607053	0.5038	0.7236	452115	0.6929	6.73E-03	2.69E-05		2	2.00E-05	1.3E+00	0.1289091
	3	0.0273	0.0076	0.0436	11192	0.0093	0.7236	452115	1.8696	1.49E-02	7.32E-04		3			
	4	0.0114	0.0032	0.0182	3368.4	0.0028	0.4784	342425	1.4614	2.36E-02	1.06E-03		4			
369	1	0.1977	0.0549	2.5267	172809	0.1434	0.7236	1E+06	9.2184	1.74E-02	4.00E-04	369	1			
	2	0.1208	0.0336	0.5145	346887	0.2879	0.7236	452115	1.1584	2.67E-02	1.87E-04		2	1.40E-04	1.3E+00	0.1251923
	3	0.0276	0.0077	0.044	15390	0.0128	0.7236	452115	1.5595	4.81E-02	1.73E-03		3			
	4	0.0114	0.0032	0.0182	3368.4	0.0028	0.4784	342425	1.4614	7.53E-02	3.39E-03		4			
371	1	0.1977	0.0549	2.5267	172809	0.1434	0.7236	1E+06	9.2184	1.26E-02	2.89E-04	371	1			
	2	0.1208	0.0336	0.5145	404702	0.3358	0.7236	452115	1.0079	1.74E-02	1.04E-04		2	9.00E-05	1.2E+00	0.0640847
	3	0.0271	0.0075	0.0434	24804	0.0208	0.7236	452115	1.1156	2.41E-02	5.30E-04		3			
	4	0.0114	0.0032	0.0182	3368.4	0.0028	0.4784	342425	1.4614	3.88E-02	1.75E-03		4			
371b	1	0.1977	0.0549	2.5267	172809	0.1434	0.7236	1E+06	9.2184	7.39E-03	1.70E-04	371b	1			
	2	0.1208	0.0336	0.5145	346887	0.2879	0.7236	452115	1.1584	1.13E-02	7.93E-05		2	7.00E-05	1.1E+00	0.0541022
	3	0.0276	0.0077	0.044	17314	0.0144	0.7236	452115	1.4464	1.92E-02	6.13E-04		3			
	4	0.0114	0.0032	0.0182	3368.4	0.0028	0.4784	342425	1.4614	3.01E-02	1.35E-03		4			
374	1	0.1977	0.0549	2.5267	172809	0.1434	0.7236	1E+06	9.2184	1.70E-02	3.90E-04	374	1			
	2	0.0926	0.0257	0.3942	265781	0.2206	0.7236	452115	1.1584	2.60E-02	1.82E-04		2	9.00E-05	2.0E+00	0.3059589
	3	0.0271	0.0075	0.0434	63452	0.0527	0.7236	452115	0.5212	1.99E-02	1.71E-04		3			
	4	0.0114	0.0032	0.0182	3368.4	0.0028	0.4784	342425	1.4614	3.39E-02	1.53E-03		4			
375	1	0.1977	0.0549	2.5267	172809	0.1434	0.7236	1E+06	9.2184	1.01E-02	2.32E-04	375	1			
	2	0.1208	0.0336	0.5145	404702	0.3358	0.7236	452115	1.0079	1.39E-02	8.36E-05		2	4.00E-05	2.1E+00	0.32027
	3	0.0276	0.0077	0.044	27702	0.023	0.7236	452115	1.0396	1.83E-02	3.65E-04		3			
	4	0.0114	0.0032	0.0182	3368.4	0.0028	0.4784	342425	1.4614	2.96E-02	1.33E-03		4			
398a	1	0.1977	0.0549	2.5267	172809	0.1434	0.7236	1E+06	9.2184	1.77E-03	4.07E-05	398a	1			
	2	0.1208	0.0336	0.5145	269801	0.2239	0.7236	452115	1.4462	3.22E-03	2.90E-05		2	1.20E-04	2.4E-01	-0.616947
	3	0.0313	0.0087	0.0501	20998	0.0174	0.7236	452115	1.3862	5.13E-03	1.54E-04		3			
	4	0.0114	0.0032	0.0182	3368.4	0.0028	0.4784	342425	1.4614	8.00E-03	3.60E-04		4			

APPENDIX VI

Final calibrated "foodweb impact model" worksheets for methyl-Hg, Zn and PCBs

THOMANN, 5 COMPARTMENT FOOD WEB MODEL [MERCURY]

Fraction of dissolved methyl-mercury in w.c. = 0.01
Fraction of dissolved methyl-mercury in s.l. = 0.01
Fraction of particulate methyl-mercury in w.c. = 0.01
Fraction of particulate methyl-mercury in s.l. = 0.01

Methyl-mercury
Water/Sediment Concs:
[Station-Specific]
Cw & Cs in ug/Lw
Rwd & Rsd in ug/kgs
Focw & Focs fractions
Rw & Rs in ug/kgoc
Pcs & Pcws in Lw/kgoc

Selection of "Ec":

	Value	Eqs LKOW range		Calc's	Calib LKOW
Eq 1 :	2.0324	2	4		
Eq 2 :	2.2476	4	4.5	2.2476	5.816
Eq 3 :	0.8	4.5	6.5	0.8	
Eq 4 :	1.0736	6.5	8	0.8	True
Eq 5 :	0.8552	8	8.5	0.8	"Ec"
Eq 6 :	0.2647	8.5	9	0.8	0.8

STN NO [1979]	TROPHIC LEVEL	W gm	LIP	A	ALF [= Ec]	BETA	GAM	DEL	FI
112	1	0.0002	0.023	0.1	0.8	0.2	0.2	0.01	0.036
	2	0.01	0.05	0.3	0.8	0.2	0.2	0.01	0.036
	3	1.8	0.036	0.8	0.8	0.2	0.2	0.01	0.036
	4	128	0.092	0.8	0.8	0.2	0.2	0.01	0.036
	5	0.016	0.016	0.2	0.8	0.2	0.2	0.01	0.036
104	1	0.0002	0.023	0.1	0.8	0.2	0.2	0.01	0.036
	2	0.01	0.05	0.3	0.8	0.2	0.2	0.01	0.036
	3	1.8	0.036	0.8	0.8	0.2	0.2	0.01	0.036
	4	128	0.092	0.8	0.8	0.2	0.2	0.01	0.036
	5	0.016	0.016	0.2	0.8	0.2	0.2	0.01	0.036
95	1	0.0002	0.023	0.1	0.8	0.2	0.2	0.01	0.036
	2	0.01	0.05	0.3	0.8	0.2	0.2	0.01	0.036
	3	1.8	0.036	0.8	0.8	0.2	0.2	0.01	0.036
	4	128	0.092	0.8	0.8	0.2	0.2	0.01	0.036
	5	0.016	0.016	0.2	0.8	0.2	0.2	0.01	0.036
71	1	0.0002	0.023	0.1	0.8	0.2	0.2	0.01	0.036
	2	0.01	0.05	0.3	0.8	0.2	0.2	0.01	0.036
	3	1.8	0.036	0.8	0.8	0.2	0.2	0.01	0.036
	4	128	0.092	0.8	0.8	0.2	0.2	0.01	0.036
	5	0.0023	0.006	0.2	0.8	0.2	0.2	0.01	0.036
[1986]									
366a	1	0.0002	0.023	0.1	0.8	0.2	0.2	0.01	0.036
	2	0.01	0.05	0.3	0.8	0.2	0.2	0.01	0.036
	3	4	0.04	0.8	0.8	0.2	0.2	0.01	0.036
	4	313	0.045	0.8	0.8	0.2	0.2	0.01	0.036
	5	0.0023	0.006	0.2	0.8	0.2	0.2	0.01	0.036
368	1	0.0002	0.023	0.1	0.8	0.2	0.2	0.01	0.036
	2	0.01	0.05	0.3	0.8	0.2	0.2	0.01	0.036
	3	4.1	0.04	0.8	0.8	0.2	0.2	0.01	0.036
	4	313	0.045	0.8	0.8	0.2	0.2	0.01	0.036
	5	0.0023	0.003	0.2	0.8	0.2	0.2	0.01	0.036
368b	1	0.0002	0.023	0.1	0.8	0.2	0.2	0.01	0.036
	2	0.01	0.05	0.3	0.8	0.2	0.2	0.01	0.036
	3	4	0.04	0.8	0.8	0.2	0.2	0.01	0.036
	4	313	0.045	0.8	0.8	0.2	0.2	0.01	0.036
	5	0.0023	0.004	0.2	0.8	0.2	0.2	0.01	0.036
369	1	0.0002	0.023	0.1	0.8	0.2	0.2	0.01	0.036
	2	0.01	0.05	0.3	0.8	0.2	0.2	0.01	0.036
	3	3.8	0.038	0.8	0.8	0.2	0.2	0.01	0.036
	4	313	0.045	0.8	0.8	0.2	0.2	0.01	0.036
	5	0.0023	0.007	0.2	0.8	0.2	0.2	0.01	0.036
371	1	0.0002	0.023	0.1	0.8	0.2	0.2	0.01	0.036
	2	0.01	0.05	0.3	0.8	0.2	0.2	0.01	0.036
	3	4.1	0.04	0.8	0.8	0.2	0.2	0.01	0.036
	4	313	0.045	0.8	0.8	0.2	0.2	0.01	0.036
	5	0.0023	0.006	0.2	0.8	0.2	0.2	0.01	0.036
371b	1	0.0002	0.023	0.1	0.8	0.2	0.2	0.01	0.036
	2	0.01	0.05	0.3	0.8	0.2	0.2	0.01	0.036
	3	3.8	0.038	0.8	0.8	0.2	0.2	0.01	0.036
	4	313	0.045	0.8	0.8	0.2	0.2	0.01	0.036
	5	0.0023	0.007	0.2	0.8	0.2	0.2	0.01	0.036
374	1	0.0002	0.023	0.1	0.8	0.2	0.2	0.01	0.036
	2	0.01	0.05	0.3	0.8	0.2	0.2	0.01	0.036
	3	4.1	0.04	0.8	0.8	0.2	0.2	0.01	0.036
	4	313	0.045	0.8	0.8	0.2	0.2	0.01	0.036
	5	0.0089	0.007	0.2	0.8	0.2	0.2	0.01	0.036
375	1	0.0002	0.023	0.1	0.8	0.2	0.2	0.01	0.036
	2	0.01	0.05	0.3	0.8	0.2	0.2	0.01	0.036
	3	3.8	0.038	0.8	0.8	0.2	0.2	0.01	0.036
	4	313	0.045	0.8	0.8	0.2	0.2	0.01	0.036
	5	0.0023	0.006	0.2	0.8	0.2	0.2	0.01	0.036

STN NO [1979]	TROPHIC LEVEL	AWD	AOC	AC	K1 1/day					cO2 kg/L
112	1	10	2.67	0.45	0.0181	Cw	0.0024	Focw	0.095	8.50E-06
	2	5	2.67	0.45	0.0181	Cs		Focs	0.019	
	3	4	2.67	0.45	0.0181	Rwd		Rw	0	
	4	4	2.67	0.45	0.0181	Rsd	60	Rs	3157.9	
	5	7	2.67	0.45	0.0181	Pcs	ERR	Pcws	1E+06	
104	1	10	2.67	0.45	0.0181	Cw	0.0029	Focw	0.1875	8.50E-06
	2	5	2.67	0.45	0.0181	Cs	0.0097	Focs	0.0375	
	3	4	2.67	0.45	0.0181	Rwd	69.05	Rw	368.27	
	4	4	2.67	0.45	0.0181	Rsd	1.2141	Rs	32.377	
	5	7	2.67	0.45	0.0181	Pcs	3350.2	Pcws	11206	
95	1	10	2.67	0.45	0.0181	Cw	0.0026	Focw	0.24	8.50E-06
	2	5	2.67	0.45	0.0181	Cs	0.0072	Focs	0.048	
	3	4	2.67	0.45	0.0181	Rwd	62.228	Rw	259.28	
	4	4	2.67	0.45	0.0181	Rsd	43.646	Rs	909.29	
	5	7	2.67	0.45	0.0181	Pcs	126679	Pcws	349233	
71	1	10	2.67	0.45	0.0181	Cw	0.0025	Focw	0.245	8.50E-06
	2	5	2.67	0.45	0.0181	Cs	0.0068	Focs	0.049	
	3	4	2.67	0.45	0.0181	Rwd	60.236	Rw	245.66	
	4	4	2.67	0.45	0.0181	Rsd	44.998	Rs	918.32	
	5	7	2.67	0.45	0.0181	Pcs	134076	Pcws	364363	
[1986]										
366a	1	10	2.67	0.45	0.0181	Cw	0.001	Focw	0.15	8.50E-06
	2	5	2.67	0.45	0.0181	Cs	0.0033	Focs	0.03	
	3	4	2.67	0.45	0.0181	Rwd	23.643	Rw	157.62	
	4	4	2.67	0.45	0.0181	Rsd	1.6536	Rs	55.121	
	5	7	2.67	0.45	0.0181	Pcs	16885	Pcws	55720	
368	1	10	2.67	0.45	0.0181	Cw	0.001	Focw	0.14	8.50E-06
	2	5	2.67	0.45	0.0181	Cs	0.0028	Focs	0.028	
	3	4	2.67	0.45	0.0181	Rwd	23.805	Rw	170.04	
	4	4	2.67	0.45	0.0181	Rsd	16.458	Rs	587.79	
	5	7	2.67	0.45	0.0181	Pcs	213394	Pcws	590130	
368b	1	10	2.67	0.45	0.0181	Cw	0.001	Focw	0.195	8.50E-06
	2	5	2.67	0.45	0.0181	Cs	0.0027	Focs	0.039	
	3	4	2.67	0.45	0.0181	Rwd	23.498	Rw	120.5	
	4	4	2.67	0.45	0.0181	Rsd	17.374	Rs	445.48	
	5	7	2.67	0.45	0.0181	Pcs	166323	Pcws	453094	
369	1	10	2.67	0.45	0.0181	Cw	0.001	Focw	0.21	8.50E-06
	2	5	2.67	0.45	0.0181	Cs	0.0033	Focs	0.042	
	3	4	2.67	0.45	0.0181	Rwd	23.894	Rw	113.78	
	4	4	2.67	0.45	0.0181	Rsd	1.0539	Rs	25.093	
	5	7	2.67	0.45	0.0181	Pcs	7554.9	Pcws	25098	
371	1	10	2.67	0.45	0.0181	Cw	0.001	Focw	0.18	8.50E-06
	2	5	2.67	0.45	0.0181	Cs	0.0032	Focs	0.036	
	3	4	2.67	0.45	0.0181	Rwd	23.53	Rw	130.72	
	4	4	2.67	0.45	0.0181	Rsd	4.2448	Rs	117.91	
	5	7	2.67	0.45	0.0181	Pcs	37369	Pcws	119766	
371b	1	10	2.67	0.45	0.0181	Cw	0.001	Focw	0.19	8.50E-06
	2	5	2.67	0.45	0.0181	Cs	0.0028	Focs	0.038	
	3	4	2.67	0.45	0.0181	Rwd	23.725	Rw	124.87	
	4	4	2.67	0.45	0.0181	Rsd	15.288	Rs	402.32	
	5	7	2.67	0.45	0.0181	Pcs	144441	Pcws	405282	
374	1	10	2.67	0.45	0.0181	Cw	0.001	Focw	0.25	8.50E-06
	2	5	2.67	0.45	0.0181	Cs	0.0033	Focs	0.05	
	3	4	2.67	0.45	0.0181	Rwd	23.548	Rw	94.193	
	4	4	2.67	0.45	0.0181	Rsd	0.5199	Rs	10.398	
	5	7	2.67	0.45	0.0181	Pcs	3158.6	Pcws	10653	
375	1	10	2.67	0.45	0.0181	Cw	0.001	Focw	0.23	8.50E-06
	2	5	2.67	0.45	0.0181	Cs	0.003	Focs	0.046	
	3	4	2.67	0.45	0.0181	Rwd	23.54	Rw	102.35	
	4	4	2.67	0.45	0.0181	Rsd	8.1598	Rs	177.39	
	5	7	2.67	0.45	0.0181	Pcs	58820	Pcws	180103	

STN NO [1979]	TROPHIC LEVEL	GROW 1/day	RESP 1/day	KU Lw/day /kglip	K 1/day	NW Lw/ kglip	IL kgl/kgl /day	G fd.ch. mult'r
112	1	0.0549	0.1977	97222	0.1666	6.29E+05		
	2	0.0251	0.0904	40903	0.0806	3.87E+05	0.3543	2.6818
	3	0.0089	0.032	25135	0.0565	3.84E+05	0.0888	0.543
	4	0.0038	0.0136	4191.9	0.0245	1.48E+05	0.0085	0.2411
	5	0.0229	0.0823	83110	0.1451	4.95E+05	1.08	5.1451
104	1	0.0549	0.1977	97222	0.1666	6.07E+05		
	2	0.0251	0.0904	40903	0.0806	3.87E+05	0.3543	2.6818
	3	0.0089	0.032	25135	0.0565	3.84E+05	0.0888	0.543
	4	0.0038	0.0136	4191.9	0.0245	1.48E+05	0.0085	0.2411
	5	0.0229	0.0823	83110	0.1451	4.95E+05	1.08	5.1451
95	1	0.0549	0.1977	97222	0.1666	5.95E+05		
	2	0.0251	0.0904	40903	0.0806	3.87E+05	0.3543	2.6818
	3	0.0089	0.032	25135	0.0565	3.84E+05	0.0888	0.543
	4	0.0038	0.0136	4191.9	0.0245	1.48E+05	0.0085	0.2411
	5	0.0229	0.0823	83110	0.1451	4.95E+05	1.08	5.1451
71	1	0.0549	0.1977	97222	0.1666	5.93E+05		
	2	0.0251	0.0904	40903	0.0806	3.87E+05	0.3543	2.6818
	3	0.0089	0.032	25135	0.0565	3.84E+05	0.0888	0.543
	4	0.0038	0.0136	4191.9	0.0245	1.48E+05	0.0085	0.2411
	5	0.0337	0.1213	326665	0.5171	5.93E+05	4.2448	6.1653
[1986]								
366a	1	0.0549	0.1977	97222	0.1666	6.16E+05		
	2	0.0251	0.0904	40903	0.0806	3.87E+05	0.3543	2.6818
	3	0.0076	0.0273	19283	0.0476	3.50E+05	0.0681	0.494
	4	0.0032	0.0114	7166.6	0.029	2.22E+05	0.0162	0.4022
	5	0.0337	0.1213	326665	0.5171	5.93E+05	4.2448	6.1653
368	1	0.0549	0.1977	97222	0.1666	6.55E+05		
	2	0.0251	0.0904	40903	0.0806	3.87E+05	0.3543	2.6818
	3	0.0075	0.0271	19188	0.0474	3.49E+05	0.0678	0.4932
	4	0.0032	0.0114	7166.6	0.029	2.22E+05	0.0162	0.4022
	5	0.0337	0.1213	653330	1.0161	6.22E+05	8.4897	6.4695
368b	1	0.0549	0.1977	97222	0.1666	6.05E+05		
	2	0.0251	0.0904	40903	0.0806	3.87E+05	0.3543	2.6818
	3	0.0076	0.0273	19283	0.0476	3.50E+05	0.0681	0.494
	4	0.0032	0.0114	7166.6	0.029	2.22E+05	0.0162	0.4022
	5	0.0337	0.1213	489997	0.7666	6.12E+05	6.3673	6.3648
369	1	0.0549	0.1977	97222	0.1666	6.01E+05		
	2	0.0251	0.0904	40903	0.0806	3.87E+05	0.3543	2.6818
	3	0.0077	0.0276	20507	0.0494	3.59E+05	0.0724	0.5074
	4	0.0032	0.0114	7166.6	0.029	2.22E+05	0.0154	0.3821
	5	0.0337	0.1213	279998	0.4458	5.84E+05	3.6384	6.0701
371	1	0.0549	0.1977	97222	0.1666	6.09E+05		
	2	0.0251	0.0904	40903	0.0806	3.87E+05	0.3543	2.6818
	3	0.0075	0.0271	19188	0.0474	3.49E+05	0.0678	0.4932
	4	0.0032	0.0114	7166.6	0.029	2.22E+05	0.0162	0.4022
	5	0.0337	0.1213	326665	0.5171	5.93E+05	4.2448	6.1653
371b	1	0.0549	0.1977	97222	0.1666	6.06E+05		
	2	0.0251	0.0904	40903	0.0806	3.87E+05	0.3543	2.6818
	3	0.0077	0.0276	20507	0.0494	3.59E+05	0.0724	0.5074
	4	0.0032	0.0114	7166.6	0.029	2.22E+05	0.0154	0.3821
	5	0.0337	0.1213	279998	0.4458	5.84E+05	3.6384	6.0701
374	1	0.0549	0.1977	97222	0.1666	5.92E+05		
	2	0.0251	0.0904	40903	0.0806	3.87E+05	0.3543	2.6818
	3	0.0075	0.0271	19188	0.0474	3.49E+05	0.0678	0.4932
	4	0.0032	0.0114	7166.6	0.029	2.22E+05	0.0162	0.4022
	5	0.0257	0.0926	213611	0.3444	5.77E+05	2.7758	5.9998
375	1	0.0549	0.1977	97222	0.1666	5.97E+05		
	2	0.0251	0.0904	40903	0.0806	3.87E+05	0.3543	2.6818
	3	0.0077	0.0276	20507	0.0494	3.59E+05	0.0724	0.5074
	4	0.0032	0.0114	7166.6	0.029	2.22E+05	0.0154	0.3821
	5	0.0337	0.1213	326665	0.5171	5.93E+05	4.2448	6.1653

CALIBRATION FACTORS

CALPHY:	1 LKOW =	5.816	B5S =	0.1	B5W = 0.9
CALSED:	1 KOW =	654636	P5S =	0.1	P51 = 0.9
			P35 =	0.5	P32 = 0.5

STN NO [1979]	TROPHIC LEVEL	Station- Specific Parameters		BSF Kgoc/Kglip	BAF Lw/Kglip	CBODY ug/kgwet	STN NO [1979]	TROPHIC LEVEL	CBODY MEASURED ug/kgwet	Predicted/ Measured "CBODY"	Log (Pred/ Meas)
112	1 PCPRIM	ERR		4.784E-01	6.295E+05	3.475E+01	112	1			
	2 ALF35	0.8 FOCB	0.4	1.577E+00	2.075E+06	2.490E+02		2			
	3 ALF5S	0.8 G(3,5)	0.543	ERR	ERR	ERR		3			
	4 ALF51	0.8 G(5,1)	4.6306	ERR	ERR	ERR		4			
	5 ILOC5	1.8782 G5S	0.8948	ERR	ERR	ERR		5			
104	1 PCPRIM	9077.7		5.414E+01	6.068E+05	4.032E+01	104	1			
	2 ALF35	0.8 FOCB	0.4	1.797E+02	2.014E+06	2.910E+02		2			
	3 ALF5S	0.8 G(3,5)	0.543	2.981E+02	3.341E+06	3.475E+02		3	70	5.0E+00	0.6958
	4 ALF51	0.8 G(5,1)	4.6306	8.509E+01	9.535E+05	2.534E+02		4			
	5 ILOC5	1.8782 G5S	0.8948	3.061E+02	3.431E+06	1.586E+02		5	10	1.6E+01	1.2003
95	1 PCPRIM	297047		1.703E+00	5.946E+05	3.561E+01	95	1	280	1.3E-01	-0.896
	2 ALF35	0.8 FOCB	0.4	5.674E+00	1.982E+06	2.580E+02		2			
	3 ALF5S	0.8 G(3,5)	0.543	9.852E+00	3.441E+06	3.225E+02		3			
	4 ALF51	0.8 G(5,1)	4.6306	2.799E+00	9.777E+05	2.342E+02		4			
	5 ILOC5	1.8782 G5S	0.8948	1.044E+01	3.648E+06	1.520E+02		5	50	3.0E+00	0.4828
71	1 PCPRIM	310954		1.629E+00	5.934E+05	3.440E+01	71	1			
	2 ALF35	0.8 FOCB	0.4	5.430E+00	1.979E+06	2.493E+02		2			
	3 ALF5S	0.8 G(3,5)	0.543	1.053E+01	3.836E+06	3.480E+02		3			
	4 ALF51	0.8 G(5,1)	5.5488	2.945E+00	1.073E+06	2.488E+02		4			
	5 ILOC5	7.3823 G5S	1.0722	1.202E+01	4.379E+06	6.621E+01		5			
[1986]							[1986]				
366a	1 PCPRIM	45301		1.105E+01	6.158E+05	1.401E+01	366a	1			
	2 ALF35	0.8 FOCB	0.4	3.658E+01	2.038E+06	1.008E+02		2			
	3 ALF5S	0.8 G(3,5)	0.494	6.164E+01	3.434E+06	1.359E+02		3	158	8.6E-01	-0.065
	4 ALF51	0.8 G(5,1)	5.5488	2.878E+01	1.604E+06	7.139E+01		4			
	5 ILOC5	7.3823 G5S	1.0722	7.548E+01	4.206E+06	2.496E+01		5	58	4.3E-01	-0.366
368	1 PCPRIM	501579		1.109E+00	6.546E+05	1.500E+01	368	1			
	2 ALF35	0.8 FOCB	0.4	3.631E+00	2.143E+06	1.067E+02		2			
	3 ALF5S	0.8 G(3,5)	0.4932	6.735E+00	3.974E+06	1.583E+02		3	124	1.3E+00	0.1062
	4 ALF51	0.8 G(5,1)	5.8226	3.085E+00	1.821E+06	8.161E+01		4			
	5 ILOC5	14.765 G5S	1.1251	8.825E+00	5.208E+06	1.556E+01		5	17	9.2E-01	-0.038
368b	1 PCPRIM	386461		1.335E+00	6.050E+05	1.368E+01	368b	1			
	2 ALF35	0.8 FOCB	0.4	4.435E+00	2.009E+06	9.878E+01		2			
	3 ALF5S	0.8 G(3,5)	0.494	8.071E+00	3.657E+06	1.438E+02		3	170	8.5E-01	-0.073
	4 ALF51	0.8 G(5,1)	5.7283	3.737E+00	1.693E+06	7.491E+01		4			
	5 ILOC5	11.073 G5S	1.1069	1.034E+01	4.685E+06	1.842E+01		5	5	3.7E+00	0.5664
369	1 PCPRIM	20369		2.396E+01	6.015E+05	1.383E+01	369	1			
	2 ALF35	0.8 FOCB	0.4	7.969E+01	2.000E+06	9.998E+01		2			
	3 ALF5S	0.8 G(3,5)	0.5074	1.363E+02	3.420E+06	1.299E+02		3	150	8.7E-01	-0.062
	4 ALF51	0.8 G(5,1)	5.4631	6.093E+01	1.529E+06	6.880E+01		4			
	5 ILOC5	6.3277 G5S	1.0557	1.606E+02	4.032E+06	2.822E+01		5	13	2.2E+00	0.3366
371	1 PCPRIM	98129		5.081E+00	6.085E+05	1.378E+01	371	1			
	2 ALF35	0.8 FOCB	0.4	1.686E+01	2.019E+06	9.938E+01		2			
	3 ALF5S	0.8 G(3,5)	0.4932	2.864E+01	3.431E+06	1.351E+02		3	126	1.1E+00	0.0303
	4 ALF51	0.8 G(5,1)	5.5488	1.338E+01	1.602E+06	7.098E+01		4			
	5 ILOC5	7.3823 G5S	1.0722	3.531E+01	4.229E+06	2.498E+01		5	24	1.0E+00	0.0174
371b	1 PCPRIM,	343289		1.496E+00	6.062E+05	1.384E+01	371b	1			
	2 ALF35	0.8 FOCB	0.4	4.966E+00	2.013E+06	9.989E+01		2			
	3 ALF5S	0.8 G(3,5)	0.5074	8.951E+00	3.628E+06	1.368E+02		3	163	8.4E-01	-0.076
	4 ALF51	0.8 G(5,1)	5.4631	3.969E+00	1.609E+06	7.185E+01		4			
	5 ILOC5	6.3277 G5S	1.0557	1.093E+01	4.429E+06	3.077E+01		5	23	1.3E+00	0.1265
374	1 PCPRIM	8551.2		5.613E+01	5.923E+05	1.342E+01	374	1			
	2 ALF35	0.8 FOCB	0.4	1.872E+02	1.975E+06	9.732E+01		2			
	3 ALF5S	0.8 G(3,5)	0.4932	3.087E+02	3.258E+06	1.284E+02		3	109	1.2E+00	0.0711
	4 ALF51	0.8 G(5,1)	5.3998	1.452E+02	1.533E+06	6.795E+01		4			
	5 ILOC5	4.8274 G5S	1.0434	3.716E+02	3.922E+06	2.705E+01		5	100	2.7E-01	-0.568
375	1 PCPRIM	149315		3.314E+00	5.969E+05	1.352E+01	375	1			
	2 ALF35	0.8 FOCB	0.4	1.104E+01	1.988E+06	9.789E+01		2			
	3 ALF5S	0.8 G(3,5)	0.5074	1.949E+01	3.509E+06	1.313E+02		3	110	1.2E+00	0.077
	4 ALF51	0.8 G(5,1)	5.5488	8.680E+00	1.583E+06	6.929E+01		4			
	5 ILOC5	7.3823 G5S	1.0722	2.343E+01	4.220E+06	2.494E+01		5	29	8.6E-01	-0.065

STATISTICAL SUMMARY OF CALIBRATION (FOR MERCURY):

		N	1979	N	1979+1986	N	1986
GEOMETRIC AVERAGE Predicted / Measured	Comp. 1	1	1.27E-01	1	1.27E-01	0	
	Comp. 2	0		0		0	
	Comp. 3	1	4.96E+00	9	1.20E+00	8	1.00E+00
	Comp. 4	0		0		0	
	Comp. 5	2	6.94E+00	10	1.48E+00	8	1.00E+00
	OVERALL	4	2.35E+00	20	1.19E+00	16	1.00E+00
S.D. (Pred/Meas)			5.9481921		3.3553153		0.7628597
S.D. (LOG[pred/meas])			0.7762131		0.4360363		0.2443201

CALPHY:	1	LKOW =	5.816	B5S =	0.1	B5W =	0.9
CALSED:	1	KOW =	6.546E+05	P5S =	0.1	P51 =	0.9
		K1 =	0.0181	P35 =	0.5	P32 =	0.5

THOMANN, 5 COMPARTMENT FOOD WEB MODEL [ZINC]

Water/Sediment Concs: [Station-Specific] Cw & Cs in ug/Lw; Rwd & Rsd in ug/kgs; Focw & Focs fractions; Rw & Rs in ug/kgoc; Pcs & Pcws in Lw/kgoc

Selection of "Ec":

	Value	Eqs LKOW range		Calc's	Calib
Eq 1 :	0.7244	2	4		LKOW
Eq 2 :	1.262	4	4.5	1.262	4.92
Eq 3 :	0.8	4.5	6.5	0.8	
Eq 4 :	1.432	6.5	8	0.8	True
Eq 5 :	1.124	8	8.5	0.8	"Ec"
Eq 6 :	0.3364	8.5	9	0.8	0.8

STN NO [1979]	TROPHIC LEVEL	W gm	LIP	A	ALF [= Ec]	BETA	GAM	DEL	FI
112	1	0.0002	0.023	0.1	0.8	0.2	0.2	0.01	0.036
	2	0.01	0.05	0.3	0.8	0.2	0.2	0.01	0.036
	3	1.8	0.036	0.8	0.8	0.2	0.2	0.01	0.036
	4	128	0.092	0.8	0.8	0.2	0.2	0.01	0.036
	5	0.016	0.016	0.2	0.8	0.2	0.2	0.01	0.036
104	1	0.0002	0.023	0.1	0.8	0.2	0.2	0.01	0.036
	2	0.01	0.05	0.3	0.8	0.2	0.2	0.01	0.036
	3	1.8	0.036	0.8	0.8	0.2	0.2	0.01	0.036
	4	128	0.092	0.8	0.8	0.2	0.2	0.01	0.036
	5	0.016	0.016	0.2	0.8	0.2	0.2	0.01	0.036
95	1	0.0002	0.023	0.1	0.8	0.2	0.2	0.01	0.036
	2	0.01	0.05	0.3	0.8	0.2	0.2	0.01	0.036
	3	1.8	0.036	0.8	0.8	0.2	0.2	0.01	0.036
	4	128	0.092	0.8	0.8	0.2	0.2	0.01	0.036
	5	0.016	0.016	0.2	0.8	0.2	0.2	0.01	0.036
71	1	0.0002	0.023	0.1	0.8	0.2	0.2	0.01	0.036
	2	0.01	0.05	0.3	0.8	0.2	0.2	0.01	0.036
	3	1.8	0.036	0.8	0.8	0.2	0.2	0.01	0.036
	4	128	0.092	0.8	0.8	0.2	0.2	0.01	0.036
	5	0.0023	0.006	0.2	0.8	0.2	0.2	0.01	0.036
[1986] 366a	1	0.0002	0.023	0.1	0.8	0.2	0.2	0.01	0.036
	2	0.01	0.05	0.3	0.8	0.2	0.2	0.01	0.036
	3	4	0.04	0.8	0.8	0.2	0.2	0.01	0.036
	4	313	0.045	0.8	0.8	0.2	0.2	0.01	0.036
	5	0.0023	0.006	0.2	0.8	0.2	0.2	0.01	0.036
368	1	0.0002	0.023	0.1	0.8	0.2	0.2	0.01	0.036
	2	0.01	0.05	0.3	0.8	0.2	0.2	0.01	0.036
	3	4.1	0.04	0.8	0.8	0.2	0.2	0.01	0.036
	4	313	0.045	0.8	0.8	0.2	0.2	0.01	0.036
	5	0.0023	0.003	0.2	0.8	0.2	0.2	0.01	0.036
368b	1	0.0002	0.023	0.1	0.8	0.2	0.2	0.01	0.036
	2	0.01	0.05	0.3	0.8	0.2	0.2	0.01	0.036
	3	4	0.04	0.8	0.8	0.2	0.2	0.01	0.036
	4	313	0.045	0.8	0.8	0.2	0.2	0.01	0.036
	5	0.0023	0.004	0.2	0.8	0.2	0.2	0.01	0.036
369	1	0.0002	0.023	0.1	0.8	0.2	0.2	0.01	0.036
	2	0.01	0.05	0.3	0.8	0.2	0.2	0.01	0.036
	3	3.8	0.038	0.8	0.8	0.2	0.2	0.01	0.036
	4	313	0.045	0.8	0.8	0.2	0.2	0.01	0.036
	5	0.0023	0.007	0.2	0.8	0.2	0.2	0.01	0.036
371	1	0.0002	0.023	0.1	0.8	0.2	0.2	0.01	0.036
	2	0.01	0.05	0.3	0.8	0.2	0.2	0.01	0.036
	3	4.1	0.04	0.8	0.8	0.2	0.2	0.01	0.036
	4	313	0.045	0.8	0.8	0.2	0.2	0.01	0.036
	5	0.0023	0.006	0.2	0.8	0.2	0.2	0.01	0.036
371b	1	0.0002	0.023	0.1	0.8	0.2	0.2	0.01	0.036
	2	0.01	0.05	0.3	0.8	0.2	0.2	0.01	0.036
	3	3.8	0.038	0.8	0.8	0.2	0.2	0.01	0.036
	4	313	0.045	0.8	0.8	0.2	0.2	0.01	0.036
	5	0.0023	0.007	0.2	0.8	0.2	0.2	0.01	0.036
374	1	0.0002	0.023	0.1	0.8	0.2	0.2	0.01	0.036
	2	0.01	0.05	0.3	0.8	0.2	0.2	0.01	0.036
	3	4.1	0.04	0.8	0.8	0.2	0.2	0.01	0.036
	4	313	0.045	0.8	0.8	0.2	0.2	0.01	0.036
	5	0.0069	0.007	0.2	0.8	0.2	0.2	0.01	0.036
375	1	0.0002	0.023	0.1	0.8	0.2	0.2	0.01	0.036
	2	0.01	0.05	0.3	0.8	0.2	0.2	0.01	0.036
	3	3.8	0.038	0.8	0.8	0.2	0.2	0.01	0.036
	4	313	0.045	0.8	0.8	0.2	0.2	0.01	0.036
	5	0.0023	0.006	0.2	0.8	0.2	0.2	0.01	0.036

STN NO [1979]	TROPHIC LEVEL	AWD	AOC	AC	K1 1/day		Water/Sediment Concs			cO2 kg/L
112	1	10	2.67	0.45	0.136	Cw	4.6	Focw	0.095	8.50E-06
	2	5	2.67	0.45	0.136	Cs		Focs	0.019	
	3	4	2.67	0.45	0.136	Rwd		Rw	0	
	4	4	2.67	0.45	0.136	Rsd	60	Rs	3157.9	
	5	7	2.67	0.45	0.136	Pcs	ERR	Pcws	686.5	
104	1	10	2.67	0.45	0.136	Cw	5.1345	Focw	0.1875	8.50E-06
	2	5	2.67	0.45	0.136	Cs	14.23	Focs	0.0375	
	3	4	2.67	0.45	0.136	Rwd	90881	Rw	484699	
	4	4	2.67	0.45	0.136	Rsd	50000	Rs	1E+06	
	5	7	2.67	0.45	0.136	Pcs	93699	Pcws	259680	
95	1	10	2.67	0.45	0.136	Cw	24.926	Focw	0.24	8.50E-06
	2	5	2.67	0.45	0.136	Cs	54.971	Focs	0.048	
	3	4	2.67	0.45	0.136	Rwd	441194	Rw	2E+06	
	4	4	2.67	0.45	0.136	Rsd	1E+06	Rs	3E+07	
	5	7	2.67	0.45	0.136	Pcs	530582	Pcws	1E+06	
71	1	10	2.67	0.45	0.136	Cw	6.7209	Focw	0.245	8.50E-06
	2	5	2.67	0.45	0.136	Cs	19.099	Focs	0.049	
	3	4	2.67	0.45	0.136	Rwd	154360	Rw	630040	
	4	4	2.67	0.45	0.136	Rsd	350000	Rs	7E+06	
	5	7	2.67	0.45	0.136	Pcs	373983	Pcws	819052	
[1986] 366a	1	10	2.67	0.45	0.136	Cw	6.1928	Focw	0.15	8.50E-06
	2	5	2.67	0.45	0.136	Cs	16.183	Focs	0.03	
	3	4	2.67	0.45	0.136	Rwd	109612	Rw	730749	
	4	4	2.67	0.45	0.136	Rsd	58000	Rs	2E+06	
	5	7	2.67	0.45	0.136	Pcs	119465	Pcws	312191	
368	1	10	2.67	0.45	0.136	Cw	22.383	Focw	0.14	8.50E-06
	2	5	2.67	0.45	0.136	Cs	49.439	Focs	0.028	
	3	4	2.67	0.45	0.136	Rwd	396176	Rw	3E+06	
	4	4	2.67	0.45	0.136	Rsd	4E+06	Rs	1E+08	
	5	7	2.67	0.45	0.136	Pcs	3E+06	Pcws	6E+06	
368b	1	10	2.67	0.45	0.136	Cw	6.7621	Focw	0.195	8.50E-06
	2	5	2.67	0.45	0.136	Cs	14.827	Focs	0.039	
	3	4	2.67	0.45	0.136	Rwd	119689	Rw	613789	
	4	4	2.67	0.45	0.136	Rsd	88000	Rs	2E+06	
	5	7	2.67	0.45	0.136	Pcs	152187	Pcws	333686	
369	1	10	2.67	0.45	0.136	Cw	28.203	Focw	0.21	8.50E-06
	2	5	2.67	0.45	0.136	Cs	75.349	Focs	0.042	
	3	4	2.67	0.45	0.136	Rwd	499194	Rw	2E+06	
	4	4	2.67	0.45	0.136	Rsd	260000	Rs	6E+06	
	5	7	2.67	0.45	0.136	Pcs	82158	Pcws	219497	
371	1	10	2.67	0.45	0.136	Cw	7.9729	Focw	0.18	8.50E-06
	2	5	2.67	0.45	0.136	Cs	19.714	Focs	0.036	
	3	4	2.67	0.45	0.136	Rwd	141120	Rw	783999	
	4	4	2.67	0.45	0.136	Rsd	240000	Rs	7E+06	
	5	7	2.67	0.45	0.136	Pcs	338164	Pcws	836169	
371b	1	10	2.67	0.45	0.136	Cw	18.425	Focw	0.19	8.50E-06
	2	5	2.67	0.45	0.136	Cs	41.003	Focs	0.038	
	3	4	2.67	0.45	0.136	Rwd	326129	Rw	2E+06	
	4	4	2.67	0.45	0.136	Rsd	74000	Rs	2E+06	
	5	7	2.67	0.45	0.136	Pcs	47493	Pcws	105890	
374	1	10	2.67	0.45	0.136	Cw	7.9518	Focw	0.25	8.50E-06
	2	5	2.67	0.45	0.136	Cs	21.857	Focs	0.05	
	3	4	2.67	0.45	0.136	Rwd	140746	Rw	562986	
	4	4	2.67	0.45	0.136	Rsd	98000	Rs	2E+06	
	5	7	2.67	0.45	0.136	Pcs	89675	Pcws	246486	
375	1	10	2.67	0.45	0.136	Cw	7.7949	Focw	0.23	8.50E-06
	2	5	2.67	0.45	0.136	Cs	18.367	Focs	0.046	
	3	4	2.67	0.45	0.136	Rwd	137971	Rw	599872	
	4	4	2.67	0.45	0.136	Rsd	300000	Rs	7E+06	
	5	7	2.67	0.45	0.136	Pcs	355077	Pcws	836662	

STN NO [1979]	TROPHIC LEVEL	GROW 1/day	RESP 1/day	KU Lw/day /kglip	K 1/day	NW Lw/ kglip	IL kgl/kgl /day	G fd.ch. mult'r
112	1	0.0549	0.1977	97222	1.3049	8.28E+04		
	2	0.0251	0.0904	40903	0.6278	6.27E+04	0.3543	0.4342
	3	0.0089	0.032	25135	0.4382	5.62E+04	0.0888	0.0794
	4	0.0038	0.0136	4191.9	0.1864	2.20E+04	0.0085	0.0359
	5	0.0229	0.0823	83110	1.1352	7.18E+04	1.08	0.7461
104	1	0.0549	0.1977	97222	1.3049	8.24E+04		
	2	0.0251	0.0904	40903	0.6278	6.27E+04	0.3543	0.4342
	3	0.0089	0.032	25135	0.4382	5.62E+04	0.0888	0.0794
	4	0.0038	0.0136	4191.9	0.1864	2.20E+04	0.0085	0.0359
	5	0.0229	0.0823	83110	1.1352	7.18E+04	1.08	0.7461
95	1	0.0549	0.1977	97222	1.3049	8.21E+04		
	2	0.0251	0.0904	40903	0.6278	6.27E+04	0.3543	0.4342
	3	0.0089	0.032	25135	0.4382	5.62E+04	0.0888	0.0794
	4	0.0038	0.0136	4191.9	0.1864	2.20E+04	0.0085	0.0359
	5	0.0229	0.0823	83110	1.1352	7.18E+04	1.08	0.7461
71	1	0.0549	0.1977	97222	1.3049	8.21E+04		
	2	0.0251	0.0904	40903	0.6278	6.27E+04	0.3543	0.4342
	3	0.0089	0.032	25135	0.4382	5.62E+04	0.0888	0.0794
	4	0.0038	0.0136	4191.9	0.1864	2.20E+04	0.0085	0.0359
	5	0.0337	0.1213	326665	4.0634	7.97E+04	4.2448	0.8289
[1986] 366a	1	0.0549	0.1977	97222	1.3049	8.25E+04		
	2	0.0251	0.0904	40903	0.6278	6.27E+04	0.3543	0.4342
	3	0.0076	0.0273	19283	0.3678	5.14E+04	0.0681	0.0725
	4	0.0032	0.0114	7166.6	0.2222	3.18E+04	0.0162	0.0578
	5	0.0337	0.1213	326665	4.0634	7.97E+04	4.2448	0.8289
368	1	0.0549	0.1977	97222	1.3049	8.32E+04		
	2	0.0251	0.0904	40903	0.6278	6.27E+04	0.3543	0.4342
	3	0.0075	0.0271	19188	0.3667	5.13E+04	0.0678	0.0724
	4	0.0032	0.0114	7166.6	0.2222	3.18E+04	0.0162	0.0575
	5	0.0337	0.1213	653330	7.9906	8.14E+04	8.4897	0.8464
368b	1	0.0549	0.1977	97222	1.3049	8.23E+04		
	2	0.0251	0.0904	40903	0.6278	6.27E+04	0.3543	0.4342
	3	0.0076	0.0273	19283	0.3678	5.14E+04	0.0681	0.0725
	4	0.0032	0.0114	7166.6	0.2222	3.18E+04	0.0162	0.0575
	5	0.0337	0.1213	489997	6.0271	8.08E+04	6.3673	0.8405
369	1	0.0549	0.1977	97222	1.3049	8.23E+04		
	2	0.0251	0.0904	40903	0.6278	6.27E+04	0.3543	0.4342
	3	0.0077	0.0276	20507	0.3825	5.26E+04	0.0724	0.0742
	4	0.0032	0.0114	7166.6	0.2222	3.18E+04	0.0154	0.0546
	5	0.0337	0.1213	279998	3.5023	7.92E+04	3.6384	0.8232
371	1	0.0549	0.1977	97222	1.3049	8.24E+04		
	2	0.0251	0.0904	40903	0.6278	6.27E+04	0.3543	0.4342
	3	0.0075	0.0271	19188	0.3667	5.13E+04	0.0678	0.0724
	4	0.0032	0.0114	7166.6	0.2222	3.18E+04	0.0162	0.0575
	5	0.0337	0.1213	326665	4.0634	7.97E+04	4.2448	0.8289
371b	1	0.0549	0.1977	97222	1.3049	8.23E+04		
	2	0.0251	0.0904	40903	0.6278	6.27E+04	0.3543	0.4342
	3	0.0077	0.0276	20507	0.3825	5.26E+04	0.0724	0.0742
	4	0.0032	0.0114	7166.6	0.2222	3.18E+04	0.0154	0.0546
	5	0.0337	0.1213	279998	3.5023	7.92E+04	3.6384	0.8232
374	1	0.0549	0.1977	97222	1.3049	8.21E+04		
	2	0.0251	0.0904	40903	0.6278	6.27E+04	0.3543	0.4342
	3	0.0075	0.0271	19188	0.3667	5.13E+04	0.0678	0.0724
	4	0.0032	0.0114	7166.6	0.2222	3.18E+04	0.0162	0.0575
	5	0.0257	0.0926	213611	2.7042	7.82E+04	2.7758	0.8134
375	1	0.0549	0.1977	97222	1.3049	8.22E+04		
	2	0.0251	0.0904	40903	0.6278	6.27E+04	0.3543	0.4342
	3	0.0077	0.0276	20507	0.3825	5.26E+04	0.0724	0.0742
	4	0.0032	0.0114	7166.6	0.2222	3.18E+04	0.0154	0.0546
	5	0.0337	0.1213	326665	4.0634	7.97E+04	4.2448	0.8289

CALIBRATION FACTORS

CALPHY:	1 LKOW = 4.92	B5S =	0.1	B5W =	0.9
CALSED:	1 KOW = 83176	P5S =	0.1	P51 =	0.9
		P35 =	0.5	P32 =	0.5

STN NO [1979]	TROPHIC LEVEL	Station-Specific Parameters		BSF Kgoc/Kglip	BAF Lw/Kglip	CBODY ug/kgwet	STN NO [1979]	TROPHIC LEVEL	CBODY MEASURED ug/kgwet	Predicted/ Measured "CBODY"	Log (Pred/ Meas)
112	1 PCPRIM	ERR		1.205E+02	8.276E+04	8.756E+03	112	1	81000		
	2 ALF35	0.8 FOCB	0.4	1.436E+02	9.858E+04	2.267E+04		2			
	3 ALF5S	0.8 G(3,5)	0.0794	ERR	ERR	ERR		3			
	4 ALF51	0.8 G(5,1)	0.6714	ERR	ERR	ERR		4			
	5 ILOC5	1.8782 G5S	0.1297	ERR	ERR	ERR		5	78000		
104	1 PCPRIM	220602		3.171E-01	8.235E+04	9.725E+03	104	1			
	2 ALF35	0.8 FOCB	0.4	3.790E-01	9.841E+04	2.526E+04		2			
	3 ALF5S	0.8 G(3,5)	0.0794	2.996E-01	7.781E+04	1.438E+04		3			
	4 ALF51	0.8 G(5,1)	0.6714	9.562E-02	2.483E+04	1.173E+04		4			
	5 ILOC5	1.8782 G5S	0.1297	6.680E-01	1.735E+05	1.425E+04		5	32000	4.5E-01	-0.351
95	1 PCPRIM	1E+06		7.018E-02	8.212E+04	4.708E+04	95	1	450000	1.0E-01	-0.98
	2 ALF35	0.8 FOCB	0.4	8.401E-02	9.831E+04	1.225E+05		2			
	3 ALF5S	0.8 G(3,5)	0.0794	7.422E-02	8.685E+04	7.793E+04		3			
	4 ALF51	0.8 G(5,1)	0.6714	2.150E-02	2.516E+04	5.769E+04		4			
	5.ILOC5	1.8782 G5S	0.1297	2.456E-01	2.874E+05	1.146E+05		5	150000	7.6E-01	-0.117
71	1 PCPRIM	731945		1.002E-01	8.210E+04	1.647E+04	71	1			
	2 ALF35	0.8 FOCB	0.4	1.200E-01	9.830E+04	4.286E+04		2			
	3 ALF5S	0.8 G(3,5)	0.0794	1.042E-01	8.535E+04	2.680E+04		3			
	4 ALF51	0.8 G(5,1)	0.746	3.065E-02	2.510E+04	2.014E+04		4			
	5 ILOC5	7.3823 G5S	0.1441	3.279E-01	2.685E+05	1.405E+04		5	49000	2.9E-01	-0.542
[1986]							[1986]				
366a	1 PCPRIM	268823		2.643E-01	8.251E+04	1.175E+04	366a	1			
	2 ALF35	0.8 FOCB	0.4	3.154E-01	9.848E+04	3.049E+04		2			
	3 ALF5S	0.8 G(3,5)	0.0725	2.337E-01	7.296E+04	1.807E+04		3	33000	5.5E-01	-0.261
	4 ALF51	0.8 G(5,1)	0.746	1.153E-01	3.600E+04	1.003E+04		4			
	5 ILOC5	7.3823 G5S	0.1441	6.379E-01	1.991E+05	7.400E+03		5	10000	7.4E-01	-0.131
368	1 PCPRIM	5E+06		1.372E-02	8.318E+04	4.282E+04	368	1			
	2 ALF35	0.8 FOCB	0.4	1.629E-02	9.876E+04	1.105E+05		2			
	3 ALF5S	0.8 G(3,5)	0.0724	2.214E-02	1.343E+05	1.202E+05		3	43000	2.8E+00	0.4464
	4 ALF51	0.8 G(5,1)	0.7617	6.519E-03	3.952E+04	3.981E+04		4			
	5 ILOC5	14.765 G5S	0.1472	1.727E-01	1.047E+06	7.031E+04		5	23000	3.1E+00	0.4853
368b	1 PCPRIM	298131		2.467E-01	8.232E+04	1.280E+04	368b	1			
	2 ALF35	0.8 FOCB	0.4	2.949E-01	9.839E+04	3.327E+04		2			
	3 ALF5S	0.8 G(3,5)	0.0725	2.191E-01	7.312E+04	1.978E+04		3	27000	7.3E-01	-0.135
	4 ALF51	0.8 G(5,1)	0.7564	1.079E-01	3.601E+04	1.096E+04		4			
	5 ILOC5	11.073 G5S	0.1462	6.039E-01	2.015E+05	5.451E+03		5	13000	4.2E-01	-0.377
369	1 PCPRIM	188060		3.747E-01	8.225E+04	5.335E+04	369	1			
	2 ALF35	0.8 FOCB	0.4	4.481E-01	9.836E+04	1.387E+05		2			
	3 ALF5S	0.8 G(3,5)	0.0742	3.352E-01	7.357E+04	7.885E+04		3	31000	2.5E+00	0.4054
	4 ALF51	0.8 G(5,1)	0.7409	1.632E-01	3.582E+04	4,547E+04		4			
	5 ILOC5	6.3277 G5S	0.1432	8.418E-01	1.848E+05	3.648E+04		5	16000	2.3E+00	0.3579
371	1 PCPRIM	728835		9.852E-02	8.238E+04	1.511E+04	371	1			
	2 ALF35	0.8 FOCB	0.4	1.177E-01	9.842E+04	3.923E+04		2			
	3 ALF5S	0.8 G(3,5)	0.0724	9.353E-02	7.820E+04	2.494E+04		3	38000	6.6E-01	-0.183
	4 ALF51	0.8 G(5,1)	0.746	4.341E-02	3.630E+04	1.302E+04		4			
	5 ILOC5	7.3823 G5S	0.1441	3.270E-01	2.735E+05	1.308E+04		5	14000	9.3E-01	-0.029
371b	1 PCPRIM	94153		7.791E-01	8.234E+04	3.489E+04	371b	1			
	2 ALF35	0.8 FOCB	0.4	9.310E-01	9.840E+04	9.065E+04		2			
	3 ALF5S	0.8 G(3,5)	0.0742	6.823E-01	7.211E+04	5.049E+04		3	42000	1.2E+00	0.0799
	4 ALF51	0.8 G(5,1)	0.7409	3.382E-01	3.574E+04	2.964E+04		4			
	5 ILOC5	6.3277 G5S	0.1432	1.561E+00	1.650E+05	2.128E+04		5	10000	2.1E+00	0.328
374	1 PCPRIM	209799		3.330E-01	8.208E+04	1.501E+04	374	1			
	2 ALF35	0.8 FOCB	0.4	3.988E-01	9.829E+04	3.908E+04		2			
	3 ALF5S	0.8 G(3,5)	0.0724	2.918E-01	7.193E+04	2.288E+04		3	26000	8.8E-01	-0.056
	4 ALF51	0.8 G(5,1)	0.7321	1.458E-01	3.594E+04	1.286E+04		4			
	5 ILOC5	4.8274 G5S	0.1415	7.582E-01	1.869E+05	1.040E+04		5	35000	3.0E-01	-0.527
375	1 PCPRIM	736739		9.821E-02	8.217E+04	1.473E+04	375	1			
	2 ALF35	0.8 FOCB	0.4	1.175E-01	9.833E+04	3.832E+04		2			
	3 ALF5S	0.8 G(3,5)	0.0742	9.571E-02	8.008E+04	2.372E+04		3	47000	5.0E-01	-0.297
	4 ALF51	0.8 G(5,1)	0.746	4.324E-02	3.618E+04	1.269E+04		4			
	5 ILOC5	7.3823 G5S	0.1441	3.256E-01	2.724E+05	1.274E+04		5	16000	8.0E-01	-0.099

STATISTICAL SUMMARY OF CALIBRATION (FOR ZINC):

		N	1979	N	1979+1986	N	1986
GEOMETRIC AVERAGE	Comp. 1	1	1.05E-01	1	1.05E-01	0	
Predicted	Comp. 2	0		0		0	
----------	Comp. 3	0		8	1.00E+00	8	1.00E+00
Measured	Comp. 4	0		0		0	
	Comp. 5	3	4.61E-01	11	8.11E-01	8	1.00E+00
	OVERALL	4	3.18E-01	20	7.96E-01	16	1.00E+00
S.D. (Pred/Meas)			0.2422191		0.8898943		0.9053432
S.D. (LOG[pred/meas])			0.3167962		0.3671754		0.3062459

CALPHY:	1	LKOW =	4.92	B5S =	0.1	B5W =	0.9
CALSED:	1	KOW =	8.318E+04	P5S =	0.1	P51 =	0.9
		K1 =	0.136	P35 =	0.5	P32 =	0.5

THOMANN, 5 COMPARTMENT FOOD WEB MODEL [PCBs]

Selection of "Ec":	Value	Eqs LKOW range		Calc's	Calib LKOW
Eq 1 :	2.0965	2	4		
Eq 2 :	2.2773	4	4.5	2.2773	5.843
Eq 3 :	0.8	4.5	6.5	0.8	
Eq 4 :	1.0628	6.5	8	0.8	True
Eq 5 :	0.8471	8	8.5	0.8	"Ec"
Eq 6 :	0.2626	8.5	9	0.8	0.8

STN NO [1979]	TROPHIC LEVEL	W gm	LIP	A	ALF [= Ec]	BETA	GAM	DEL	FI
112	1	0.0002	0.023	0.1	0.8	0.2	0.2	0.01	0.036
	2	0.01	0.05	0.3	0.8	0.2	0.2	0.01	0.036
	3	1.8	0.036	0.8	0.8	0.2	0.2	0.01	0.036
	4	128	0.092	0.8	0.8	0.2	0.2	0.01	0.036
	5	0.016	0.016	0.2	0.8	0.2	0.2	0.01	0.036
104	1	0.0002	0.023	0.1	0.8	0.2	0.2	0.01	0.036
	2	0.01	0.05	0.3	0.8	0.2	0.2	0.01	0.036
	3	1.8	0.036	0.8	0.8	0.2	0.2	0.01	0.036
	4	128	0.092	0.8	0.8	0.2	0.2	0.01	0.036
	5	0.016	0.016	0.2	0.8	0.2	0.2	0.01	0.036
95	1	0.0002	0.023	0.1	0.8	0.2	0.2	0.01	0.036
	2	0.01	0.05	0.3	0.8	0.2	0.2	0.01	0.036
	3	1.8	0.036	0.8	0.8	0.2	0.2	0.01	0.036
	4	128	0.092	0.8	0.8	0.2	0.2	0.01	0.036
	5	0.016	0.016	0.2	0.8	0.2	0.2	0.01	0.036
71	1	0.0002	0.023	0.1	0.8	0.2	0.2	0.01	0.036
	2	0.01	0.05	0.3	0.8	0.2	0.2	0.01	0.036
	3	1.8	0.036	0.8	0.8	0.2	0.2	0.01	0.036
	4	128	0.092	0.8	0.8	0.2	0.2	0.01	0.036
	5	0.0023	0.006	0.2	0.8	0.2	0.2	0.01	0.036
[1986] 366a	1	0.0002	0.023	0.1	0.8	0.2	0.2	0.01	0.036
	2	0.01	0.05	0.3	0.8	0.2	0.2	0.01	0.036
	3	4	0.04	0.8	0.8	0.2	0.2	0.01	0.036
	4	313	0.045	0.8	0.8	0.2	0.2	0.01	0.036
	5	0.0023	0.006	0.2	0.8	0.2	0.2	0.01	0.036
368	1	0.0002	0.023	0.1	0.8	0.2	0.2	0.01	0.036
	2	0.01	0.05	0.3	0.8	0.2	0.2	0.01	0.036
	3	4.1	0.04	0.8	0.8	0.2	0.2	0.01	0.036
	4	313	0.045	0.8	0.8	0.2	0.2	0.01	0.036
	5	0.0023	0.003	0.2	0.8	0.2	0.2	0.01	0.036
368b	1	0.0002	0.023	0.1	0.8	0.2	0.2	0.01	0.036
	2	0.01	0.05	0.3	0.8	0.2	0.2	0.01	0.036
	3	4	0.04	0.8	0.8	0.2	0.2	0.01	0.036
	4	313	0.045	0.8	0.8	0.2	0.2	0.01	0.036
	5	0.0023	0.004	0.2	0.8	0.2	0.2	0.01	0.036
369	1	0.0002	0.023	0.1	0.8	0.2	0.2	0.01	0.036
	2	0.01	0.05	0.3	0.8	0.2	0.2	0.01	0.036
	3	3.8	0.038	0.8	0.8	0.2	0.2	0.01	0.036
	4	313	0.045	0.8	0.8	0.2	0.2	0.01	0.036
	5	0.0023	0.007	0.2	0.8	0.2	0.2	0.01	0.036
371	1	0.0002	0.023	0.1	0.8	0.2	0.2	0.01	0.036
	2	0.01	0.05	0.3	0.8	0.2	0.2	0.01	0.036
	3	4.1	0.04	0.8	0.8	0.2	0.2	0.01	0.036
	4	313	0.045	0.8	0.8	0.2	0.2	0.01	0.036
	5	0.0023	0.006	0.2	0.8	0.2	0.2	0.01	0.036
371b	1	0.0002	0.023	0.1	0.8	0.2	0.2	0.01	0.036
	2	0.01	0.05	0.3	0.8	0.2	0.2	0.01	0.036
	3	3.8	0.038	0.8	0.8	0.2	0.2	0.01	0.036
	4	313	0.045	0.8	0.8	0.2	0.2	0.01	0.036
	5	0.0023	0.007	0.2	0.8	0.2	0.2	0.01	0.036
374	1	0.0002	0.023	0.1	0.8	0.2	0.2	0.01	0.036
	2	0.01	0.05	0.3	0.8	0.2	0.2	0.01	0.036
	3	4.1	0.04	0.8	0.8	0.2	0.2	0.01	0.036
	4	313	0.045	0.8	0.8	0.2	0.2	0.01	0.036
	5	0.0089	0.007	0.2	0.8	0.2	0.2	0.01	0.036
375	1	0.0002	0.023	0.1	0.8	0.2	0.2	0.01	0.036
	2	0.01	0.05	0.3	0.8	0.2	0.2	0.01	0.036
	3	3.8	0.038	0.8	0.8	0.2	0.2	0.01	0.036
	4	313	0.045	0.8	0.8	0.2	0.2	0.01	0.036
	5	0.0023	0.006	0.2	0.8	0.2	0.2	0.01	0.036

Water/Sediment Concs:
[Station-Specific]
Cw & Cs in ug/Lw
Rwd & Rsd in ug/kgs
Focw & Focs fractions
Rw & Rs in ug/kgoc
Pcs & Pcws in Lw/kgoc

STN NO [1979]	TROPHIC LEVEL	AWD	AOC	AC	K1 1/day					cO2 kg/L
112	1	10	2.67	0.45	0	Cw	0.0009	Focw	0.095	8.50E-06
	2	5	2.67	0.45	0	Cs		Focs	0.019	
	3	4	2.67	0.45	0	Rwd		Rw	0	
	4	4	2.67	0.45	0	Rsd	60	Rs	3157.9	
	5	7	2.67	0.45	0	Pcs	ERR	Pcws	4E+06	
104	1	10	2.67	0.45	0	Cw	0.0016	Focw	0.1875	8.50E-06
	2	5	2.67	0.45	0	Cs	0.0138	Focs	0.0375	
	3	4	2.67	0.45	0	Rwd	285.21	Rw	1521.1	
	4	4	2.67	0.45	0	Rsd	50	Rs	1333.3	
	5	7	2.67	0.45	0	Pcs	96461	Pcws	822786	
95	1	10	2.67	0.45	0	Cw	0.0011	Focw	0.24	8.50E-06
	2	5	2.67	0.45	0	Cs	0.0038	Focs	0.048	
	3	4	2.67	0.45	0	Rwd	199.22	Rw	830.06	
	4	4	2.67	0.45	0	Rsd	100	Rs	2083.3	
	5	7	2.67	0.45	0	Pcs	550097	Pcws	2E+06	
71	1	10	2.67	0.45	0	Cw	0.0011	Focw	0.245	8.50E-06
	2	5	2.67	0.45	0	Cs	0.0034	Focs	0.049	
	3	4	2.67	0.45	0	Rwd	185.35	Rw	756.55	
	4	4	2.67	0.45	0	Rsd	10	Rs	204.08	
	5	7	2.67	0.45	0	Pcs	60772	Pcws	193782	
[1986] 366a	1	10	2.67	0.45	0	Cw	0.0019	Focw	0.15	8.50E-06
	2	5	2.67	0.45	0	Cs	0.0146	Focs	0.03	
	3	4	2.67	0.45	0	Rwd	331	Rw	2206.7	
	4	4	2.67	0.45	0	Rsd	60	Rs	2000	
	5	7	2.67	0.45	0	Pcs	137371	Pcws	1E+06	
368	1	10	2.67	0.45	0	Cw	0.0018	Focw	0.14	8.50E-06
	2	5	2.67	0.45	0	Cs	0.006	Focs	0.028	
	3	4	2.67	0.45	0	Rwd	311.17	Rw	2222.7	
	4	4	2.67	0.45	0	Rsd	1010	Rs	36071	
	5	7	2.67	0.45	0	Pcs	6E+06	Pcws	2E+07	
368b	1	10	2.67	0.45	0	Cw	0.0016	Focw	0.195	8.50E-06
	2	5	2.67	0.45	0	Cs	0.0052	Focs	0.039	
	3	4	2.67	0.45	0	Rwd	286.21	Rw	1467.7	
	4	4	2.67	0.45	0	Rsd	45	Rs	1153.8	
	5	7	2.67	0.45	0	Pcs	220744	Pcws	709541	
369	1	10	2.67	0.45	0	Cw	0.0018	Focw	0.21	8.50E-06
	2	5	2.67	0.45	0	Cs	0.0144	Focs	0.042	
	3	4	2.67	0.45	0	Rwd	313.25	Rw	1491.7	
	4	4	2.67	0.45	0	Rsd	85	Rs	2023.8	
	5	7	2.67	0.45	0	Pcs	140168	Pcws	1E+06	
371	1	10	2.67	0.45	0	Cw	0.0016	Focw	0.18	8.50E-06
	2	5	2.67	0.45	0	Cs	0.0104	Focs	0.036	
	3	4	2.67	0.45	0	Rwd	284.72	Rw	1581.8	
	4	4	2.67	0.45	0	Rsd	60	Rs	1666.7	
	5	7	2.67	0.45	0	Pcs	159783	Pcws	1E+06	
371b	1	10	2.67	0.45	0	Cw	0.0017	Focw	0.19	8.50E-06
	2	5	2.67	0.45	0	Cs	0.0061	Focs	0.038	
	3	4	2.67	0.45	0	Rwd	303.15	Rw	1595.5	
	4	4	2.67	0.45	0	Rsd	40	Rs	1052.6	
	5	7	2.67	0.45	0	Pcs	171741	Pcws	611123	
374	1	10	2.67	0.45	0	Cw	0.0017	Focw	0.25	8.50E-06
	2	5	2.67	0.45	0	Cs	0.0141	Focs	0.05	
	3	4	2.67	0.45	0	Rwd	292.92	Rw	1171.7	
	4	4	2.67	0.45	0	Rsd	20	Rs	400	
	5	7	2.67	0.45	0	Pcs	28422	Pcws	240339	
375	1	10	2.67	0.45	0	Cw	0.0016	Focw	0.23	8.50E-06
	2	5	2.67	0.45	0	Cs	0.0084	Focs	0.046	
	3	4	2.67	0.45	0	Rwd	289.48	Rw	1258.6	
	4	4	2.67	0.45	0	Rsd	85	Rs	1847.8	
	5	7	2.67	0.45	0	Pcs	220973	Pcws	1E+06	

STN NO [1979]	TROPHIC LEVEL	GROW 1/day	RESP 1/day	KU Lw/day /kglip	K 1/day	NW Lw/ kglip	IL kgl/kgl /day	G fd.ch. mult'r
112	1	0.0549	0.1977	97222	0.1396	6.68E+05		
	2	0.0251	0.0904	40903	0.0587	4.88E+05	0.3543	3.3813
	3	0.0089	0.032	25135	0.0361	5.59E+05	0.0888	0.7894
	4	0.0038	0.0136	4191.9	0.006	4.27E+05	0.0085	0.6955
	5	0.0229	0.0823	83110	0.1193	5.85E+05	1.08	6.0771
104	1	0.0549	0.1977	97222	0.1396	6.43E+05		
	2	0.0251	0.0904	40903	0.0587	4.88E+05	0.3543	3.3813
	3	0.0089	0.032	25135	0.0361	5.59E+05	0.0888	0.7894
	4	0.0038	0.0136	4191.9	0.006	4.27E+05	0.0085	0.6955
	5	0.0229	0.0823	83110	0.1193	5.85E+05	1.08	6.0771
95	1	0.0549	0.1977	97222	0.1396	6.29E+05		
	2	0.0251	0.0904	40903	0.0587	4.88E+05	0.3543	3.3813
	3	0.0089	0.032	25135	0.0361	5.59E+05	0.0888	0.7894
	4	0.0038	0.0136	4191.9	0.006	4.27E+05	0.0085	0.6955
	5	0.0229	0.0823	83110	0.1193	5.85E+05	1.08	6.0771
71	1	0.0549	0.1977	97222	0.1396	6.28E+05		
	2	0.0251	0.0904	40903	0.0587	4.88E+05	0.3543	3.3813
	3	0.0089	0.032	25135	0.0361	5.59E+05	0.0888	0.7894
	4	0.0038	0.0136	4191.9	0.006	4.27E+05	0.0085	0.6955
	5	0.0337	0.1213	326665	0.4689	6.50E+05	4.2448	6.7563
[1986] 366a	1	0.0549	0.1977	97222	0.1396	6.53E+05		
	2	0.0251	0.0904	40903	0.0587	4.88E+05	0.3543	3.3813
	3	0.0076	0.0273	19283	0.0277	5.47E+05	0.0681	0.7725
	4	0.0032	0.0114	7166.6	0.0103	5.33E+05	0.0162	0.9629
	5	0.0337	0.1213	326665	0.4689	6.50E+05	4.2448	6.7563
368	1	0.0549	0.1977	97222	0.1396	6.56E+05		
	2	0.0251	0.0904	40903	0.0587	4.88E+05	0.3543	3.3813
	3	0.0075	0.0271	19188	0.0275	5.47E+05	0.0678	0.7725
	4	0.0032	0.0114	7166.6	0.0103	5.33E+05	0.0162	0.9629
	5	0.0337	0.1213	653330	0.9378	6.72E+05	8.4897	6.9906
368b	1	0.0549	0.1977	97222	0.1396	6.41E+05		
	2	0.0251	0.0904	40903	0.0587	4.88E+05	0.3543	3.3813
	3	0.0076	0.0273	19283	0.0277	5.47E+05	0.0681	0.7725
	4	0.0032	0.0114	7166.6	0.0103	5.33E+05	0.0162	0.9629
	5	0.0337	0.1213	489997	0.7034	6.65E+05	6.3673	6.9107
369	1	0.0549	0.1977	97222	0.1396	6.37E+05		
	2	0.0251	0.0904	40903	0.0587	4.88E+05	0.3543	3.3813
	3	0.0077	0.0276	20507	0.0294	5.53E+05	0.0724	0.7806
	4	0.0032	0.0114	7166.6	0.0103	5.33E+05	0.0154	0.9147
	5	0.0337	0.1213	279998	0.4019	6.43E+05	3.6384	6.6816
371	1	0.0549	0.1977	97222	0.1396	6.45E+05		
	2	0.0251	0.0904	40903	0.0587	4.88E+05	0.3543	3.3813
	3	0.0075	0.0271	19188	0.0275	5.47E+05	0.0678	0.7725
	4	0.0032	0.0114	7166.6	0.0103	5.33E+05	0.0162	0.9629
	5	0.0337	0.1213	326665	0.4689	6.50E+05	4.2448	6.7563
371b	1	0.0549	0.1977	97222	0.1396	6.42E+05		
	2	0.0251	0.0904	40903	0.0587	4.88E+05	0.3543	3.3813
	3	0.0077	0.0276	20507	0.0294	5.53E+05	0.0724	0.7806
	4	0.0032	0.0114	7166.6	0.0103	5.33E+05	0.0154	0.9147
	5	0.0337	0.1213	279998	0.4019	6.43E+05	3.6384	6.6816
374	1	0.0549	0.1977	97222	0.1396	6.26E+05		
	2	0.0251	0.0904	40903	0.0587	4.88E+05	0.3543	3.3813
	3	0.0075	0.0271	19188	0.0275	5.47E+05	0.0678	0.7725
	4	0.0032	0.0114	7166.6	0.0103	5.33E+05	0.0162	0.9629
	5	0.0257	0.0926	213611	0.3066	6.43E+05	2.7758	6.6816
375	1	0.0549	0.1977	97222	0.1396	6.32E+05		
	2	0.0251	0.0904	40903	0.0587	4.88E+05	0.3543	3.3813
	3	0.0077	0.0276	20507	0.0294	5.53E+05	0.0724	0.7806
	4	0.0032	0.0114	7166.6	0.0103	5.33E+05	0.0154	0.9147
	5	0.0337	0.1213	326665	0.4689	6.50E+05	4.2448	6.7563

CALIBRATION FACTORS

CALPHY:	1 LKOW = 5.843	B5S =	0.1	B5W =	0.9
CALSED:	1 KOW = 696627	P5S =	0.1	P51 =	0.9
		P35 =	0.5	P32 =	0.5

STN NO [1979]	TROPHIC LEVEL	Station-Specific Parameters			BSF Kgoc/Kglip	BAF Lw/Kglip	CBODY ug/kgwet	STN NO [1979]	TROPHIC LEVEL	CBODY MEASURED ug/kgwet	Predicted/ Measured "CBODY"	Log (Pred/ Meas)
112	1	PCPRIM	ERR		1.799E-01	6.682E+05	1.306E+01	112	1	20		
	2	ALF35	0.8 FOCB	0.4	7.395E-01	2.747E+06	1.168E+02		2			
	3	ALF5S	0.8 G(3,5)	0.7894	ERR	ERR	ERR		3			
	4	ALF51	0.8 G(5,1)	5.4694	ERR	ERR	ERR		4			
	5	ILOC5	1.8782 G5S	1.0569	ERR	ERR	ERR		5	24		
104	1	PCPRIM	469366		7.811E-01	6.427E+05	2.395E+01	104	1			
	2	ALF35	0.8 FOCB	0.4	3.234E+00	2.661E+06	2.156E+02		2			
	3	ALF5S	0.8 G(3,5)	0.7894	8.422E+00	6.930E+06	4.043E+02		3	20	2.0E+01	1.3056
	4	ALF51	0.8 G(5,1)	5.4694	6.377E+00	5.247E+06	7.823E+02		4	243	3.2E+00	0.5078
	5	ILOC5	1.8782 G5S	1.0569	6.574E+00	5.409E+06	1.403E+02		5	20	7.0E+00	0.8459
95	1	PCPRIM	1E+06		3.418E-01	6.290E+05	1.638E+01	95	1	20	8.2E-01	-0.087
	2	ALF35	0.8 FOCB	0.4	1.421E+00	2.615E+06	1.480E+02		2			
	3	ALF5S	0.8 G(3,5)	0.7894	4.045E+00	7.444E+06	3.033E+02		3			
	4	ALF51	0.8 G(5,1)	5.4694	3.045E+00	5.605E+06	5.837E+02		4			
	5	ILOC5	1.8782 G5S	1.0569	3.318E+00	6.107E+06	1.106E+02		5	20	5.5E+00	0.7428
71	1	PCPRIM	158985		3.239E+00	6.278E+05	1.521E+01	71	1			
	2	ALF35	0.8 FOCB	0.4	1.347E+01	2.611E+06	1.375E+02		2			
	3	ALF5S	0.8 G(3,5)	0.7894	3.322E+01	6.438E+06	2.441E+02		3			
	4	ALF51	0.8 G(5,1)	6.0806	2.531E+01	4.905E+06	4.753E+02		4			
	5	ILOC5	7.3823 G5S	1.175	2.496E+01	4.837E+06	3.056E+01		5	20	1.5E+00	0.1842
[1986]								[1986]				
366a	1	PCPRIM	635214		6.136E-01	6.528E+05	2.824E+01	366a	1			
	2	ALF35	0.8 FOCB	0.4	2.534E+00	2.695E+06	2.534E+02		2			
	3	ALF5S	0.8 G(3,5)	0.7725	7.053E+00	7.501E+06	5.642E+02		3			
	4	ALF51	0.8 G(5,1)	6.0806	7.292E+00	7.755E+06	6.563E+02		4			
	5	ILOC5	7.3823 G5S	1.175	5.931E+00	6.307E+06	7.117E+01		5	85	8.4E-01	-0.077
368	1	PCPRIM	2E+07		3.213E-02	6.555E+05	2.666E+01	368	1			
	2	ALF35	0.8 FOCB	0.4	1.326E-01	2.704E+06	2.391E+02		2			
	3	ALF5S	0.8 G(3,5)	0.7725	1.256E+00	2.562E+07	1.812E+03		3			
	4	ALF51	0.8 G(5,1)	6.2916	1.235E+00	2.521E+07	2.005E+03		4			
	5	ILOC5	14.765 G5S	1.2158	1.459E+00	2.976E+07	1.579E+02		5	80	2.0E+00	0.2952
368b	1	PCPRIM	580909		9.029E-01	6.407E+05	2.396E+01	368b	1			
	2	ALF35	0.8 FOCB	0.4	3.741E+00	2.654E+06	2.158E+02		2			
	3	ALF5S	0.8 G(3,5)	0.7725	9.811E+00	6.961E+06	4.528E+02		3			
	4	ALF51	0.8 G(5,1)	6.2196	1.020E+01	7.235E+06	5.295E+02		4			
	5	ILOC5	11.073 G5S	1.2019	7.962E+00	5.650E+06	3.675E+01		5	20	1.8E+00	0.2642
369	1	PCPRIM	664483		5.600E-01	6.367E+05	2.607E+01	369	1			
	2	ALF35	0.8 FOCB	0.4	2.323E+00	2.641E+06	2.350E+02		2			
	3	ALF5S	0.8 G(3,5)	0.7808	6.592E+00	7.495E+06	5.069E+02		3			
	4	ALF51	0.8 G(5,1)	6.0134	6.498E+00	7.389E+06	5.918E+02		4			
	5	ILOC5	6.3277 G5S	1.162	5.497E+00	6.250E+06	7.787E+01		5	140	5.6E-01	-0.255
371	1	PCPRIM	666922		6.257E-01	6.447E+05	2.399E+01	371	1			
	2	ALF35	0.8 FOCB	0.4	2.589E+00	2.668E+06	2.158E+02		2			
	3	ALF5S	0.8 G(3,5)	0.7725	7.130E+00	7.346E+06	4.754E+02		3			
	4	ALF51	0.8 G(5,1)	6.0806	7.383E+00	7.606E+06	5.537E+02		4			
	5	ILOC5	7.3823 G5S	1.175	5.954E+00	6.134E+06	5.954E+01		5	90	6.6E-01	-0.179
371b	1	PCPRIM	486625		1.051E+00	6.420E+05	2.543E+01	371b	1			
	2	ALF35	0.8 FOCB	0.4	4.351E+00	2.659E+06	2.290E+02		2			
	3	ALF5S	0.8 G(3,5)	0.7808	1.117E+01	6.828E+06	4.469E+02		3			
	4	ALF51	0.8 G(5,1)	6.0134	1.109E+01	6.779E+06	5.254E+02		4			
	5	ILOC5	6.3277 G5S	1.162	8.800E+00	5.378E+06	6.484E+01		5	70	9.3E-01	-0.033
374	1	PCPRIM	137682		2.607E+00	6.265E+05	2.398E+01	374	1			
	2	ALF35	0.8 FOCB	0.4	1.084E+01	2.606E+06	2.169E+02		2			
	3	ALF5S	0.8 G(3,5)	0.7725	2.726E+01	6.553E+06	4.362E+02		3			
	4	ALF51	0.8 G(5,1)	6.0134	2.847E+01	6.842E+06	5.124E+02		4			
	5	ILOC5	4.8274 G5S	1.162	2.151E+01	5.169E+06	6.021E+01		5	90	6.7E-01	-0.175
375	1	PCPRIM	797671		5.622E-01	6.316E+05	2.389E+01	375	1			
	2	ALF35	0.8 FOCB	0,4	2.335E+00	2.623E+06	2.158E+02		2			
	3	ALF5S	0.8 G(3,5)	0.7808	6.538E+00	7.346E+06	4.591E+02		3			
	4	ALF51	0.8 G(5,1)	6.0806	6.455E+00	7.252E+06	5.367E+02		4			
	5	ILOC5	7.3823 G5S	1.175	5.408E+00	6.076E+06	5.996E+01		5	40	1.5E+00	0.1758

STATISTICAL SUMMARY OF CALIBRATION (FOR PCBs):

		N	1979	N	1979+1986	N	1986
GEOMETRIC AVERAGE Predicted	Comp. 1	1	8.19E-01	1	8.19E-01	0	
	Comp. 2	0		0		0	
	Comp. 3	1	2.02E+01	1	2.02E+01	0	
Measured	Comp. 4	1	3.22E+00	1		0	
	Comp. 5	3	3.89E+00	11	1.45E+00	8	1.00E+00
	OVERALL	6	3.83E+00	14	1.78E+00	8	1.00E+00

S.D. (Pred/Meas)		6.5440413		5.0306247		0.528567
S.D. (LOG[pred/meas])		0.452811		0.4400385		0.2007527
CALPHY: 1	LKOW =	5.843	B5S =	0.1	B5W =	0.9
CALSED: 1	KOW =	6.966E+05	P5S =	0.1	P51 =	0.9
			P35 =	0.5	P32 =	0.5

APPENDIX VII

Source code listing of the Monte Carlo load allocation program

```
$LARGE
      PROGRAM MCLA3A
      CHARACTER*16 INPUT,OUTCHM(3)
      DIMENSION CCRITW(3),CCRITS(3),CCRITB(3),CRB(3),A(10,10),
     #WCF(1000),SCF(3,1000),BCF(3,1000),RBCCF(3,1000),RFRCF(1000),
     #SUMW(10),SUMS(10),SUMB(10)
      REAL LW(10,3,1000),LS(10,3,1000),LB(10,3,1000)
C
      WRITE(*,*)
      WRITE(*,*)'ENTER THE NAME OF THE INPUT DATA FILE'
      WRITE(*,*)
      READ(*,'(A)') INPUT
      WRITE(*,*)
C
C  OPEN THE I/O FILES
C
      OPEN(5,FILE=INPUT,STATUS='UNKNOWN')
C
C  READ ALL INPUT DATA
C
      READ(5,*) NCHEM,NOUTFL,NSI
      DO 9 IC=1,NCHEM
      WRITE(*,*)
      WRITE(*,601) IC
      WRITE(*,*)
      READ(*,'(A)') OUTCHM(IC)
      WRITE(*,*)
    9 CONTINUE
      READ(5,*) CCRITW
      READ(5,*) CCRITS
      READ(5,*) CCRITB
      READ(5,*) CRB
      DO 11 I=1,NOUTFL
      READ(5,*) (A(I,J),J=I,NOUTFL)
   11 CONTINUE
C  READ CHEMICAL SPECIFIC PROBABILITY FACTORS
      READ(5,*) (WCF(I),I=1,NSI)
      READ(5,*) ((SCF(I,J),I=1,NCHEM),J=1,NSI)
      READ(5,*) ((BCF(I,J),I=1,NCHEM),J=1,NSI)
      READ(5,*) ((RBCCF(I,J),I=1,NCHEM),J=1,NSI)
      READ(5,*) (RFRCF(I),I=1,NSI)
C
C  INITIALIZE CHEMICAL LOOP, "IC"
C
      DO 100 IC=1,NCHEM
C
C  INITIALIZE STATISTICAL ITERATION LOOP, "IS"
C
      DO 200 IS=1,NSI
C  SOLVE FOR THE ALLOCATED LOADS FOR OUTFALL # 1 (FURTHEST U/S)
      LW(1,IC,IS)=(CCRITW(IC)-CRB(IC)*RBCCF(IC,IS))/(A(1,1)*
     #  WCF(IS)*RFRCF(IS))
      LS(1,IC,IS)=(CCRITS(IC)*SCF(IC,IS)-CRB(IC)*RBCCF(IC,IS))/
     #  (A(1,1)*RFRCF(IS))
      LB(1,IC,IS)=(CCRITB(IC)*BCF(IC,IS)-CRB(IC)*RBCCF(IC,IS))/
     #  (A(1,1)*RFRCF(IS))
C
C  INITIALIZE OUTFALL LOOP, "IT"
C
      DO 300 IT=2,NOUTFL
      SUMW(IT)=0.
      SUMS(IT)=0.
      SUMB(IT)=0.
      ITM=IT-1
```

```
      DO 310 J=1,ITM
      SUMW(IT)=SUMW(IT)  + A(J,IT)*LW(J,IC,IS)
      SUMS(IT)=SUMS(IT)  + A(J,IT)*LS(J,IC,IS)
      SUMB(IT)=SUMB(IT)  + A(J,IT)*LB(J,IC,IS)
  310 CONTINUE
      LW(IT,IC,IS)=(CCRITW(IC)-CRB(IC)*RBCCF(IC,IS)  - SUMW(IT))/
     #   (A(IT,IT)*WCF(IS)*RFRCF(IS))
      LS(IT,IC,IS)=(CCRITS(IC)*SCF(IC,IS)  - CRB(IC)*RBCCF(IC,IS)  -
     #   SUMS(IT))/(A(IT,IT)*RFRCF(IS))
      LB(IT,IC,IS)=(CCRITB(IC)*BCF(IC,IS)  - CRB(IC)*RBCCF(IC,IS)  -
     #   SUMB(IT))/(A(IT,IT)*RFRCF(IS))
  300 CONTINUE
  200 CONTINUE
  100 CONTINUE
C
C  WRITE OUTPUT DATA
C
      DO 325 IC=1,NCHEM
      IOFILE=6+IC
      OPEN(IOFILE,FILE=OUTCHM(IC),STATUS='UNKNOWN')
      DO 350 IT=1,NOUTFL
      WRITE(IOFILE,605) IT
      DO 375 IS=1,NSI
      WRITE(IOFILE,610) LW(IT,IC,IS),LS(IT,IC,IS),LB(IT,IC,IS)
  375 CONTINUE
  350 CONTINUE
      CLOSE(IOFILE)
  325 CONTINUE
C
C  FORMAT STATEMENTS
C
  601 FORMAT(1X,'ENTER THE NAME OF THE OUTPUT FILE FOR CHEMICAL NO.',I3)
  605 FORMAT(1X,'---------------', 'OUTFALL NO. ',I5,'---------------')
  610 FORMAT(1X,3(E12.4,1X))
C
      STOP
      END
```

```
$LARGE
      PROGRAM MCLA3B
      CHARACTER*16 INPUT,OUTCHM(3)
      DIMENSION CCRITW(3),CCRITS(3),CCRITB(3),CRB(3),A(10,10),
     #WCF(1000),SCF(3,1000),BCF(3,1000),RBCCF(3,1000),RFRCF(1000)
      REAL LW(10,3,1000),LS(10,3,1000),LB(10,3,1000)
C
      WRITE(*,*)
      WRITE(*,*)'ENTER THE NAME OF THE INPUT DATA FILE'
      WRITE(*,*)
      READ(*,'(A)') INPUT
      WRITE(*,*)
C
C  OPEN THE I/O FILES
C
      OPEN(5,FILE=INPUT,STATUS='UNKNOWN')
C
C  READ ALL INPUT DATA
C
      READ(5,*) NCHEM,NOUTFL,NSI
      DO 9 IC=1,NCHEM
      WRITE(*,*)
      WRITE(*,601) IC
      WRITE(*,*)
      READ(*,'(A)') OUTCHM(IC)
      WRITE(*,*)
    9 CONTINUE
      READ(5,*) CCRITW
      READ(5,*) CCRITS
      READ(5,*) CCRITB
      READ(5,*) CRB
      DO 11 I=1,NOUTFL
      READ(5,*) (A(I,J),J=I,NOUTFL)
   11 CONTINUE
C  READ CHEMICAL SPECIFIC PROBABILITY FACTORS
      READ(5,*) (WCF(I),I=1,NSI)
      READ(5,*) ((SCF(I,J),I=1,NCHEM),J=1,NSI)
      READ(5,*) ((BCF(I,J),I=1,NCHEM),J=1,NSI)
      READ(5,*) ((RBCCF(I,J),I=1,NCHEM),J=1,NSI)
      READ(5,*) (RFRCF(I),I=1,NSI)
C
C  INITIALIZE CHEMICAL LOOP, "IC"
C
      DO 100 IC=1,NCHEM
C
C  INITIALIZE STATISTICAL ITERATION LOOP, "IS"
C
      DO 200 IS=1,NSI
C  SOLVE FOR THE ALLOCATED LOADS FOR OUTFALL # 1 (FURTHEST U/S)
      SUMW=0.
      SUMS=0.
      SUMB=0.
      NM1=NOUTFL-1
      DO 210 I=1,NM1
      SUMW=SUMW+A(I,NOUTFL)*WCF(IS)*RFRCF(IS)*A(1,1)/A(I,I)
      SUMS=SUMS+RFRCF(IS)*A(I,NOUTFL)*A(1,1)/A(I,I)
      SUMB=SUMB+RFRCF(IS)*A(I,NOUTFL)*A(1,1)/A(I,I)
  210 CONTINUE
      LW(1,IC,IS)=(CCRITW(IC)-CRB(IC)*RBCCF(IC,IS))/(A(1,1)*
     #  WCF(IS)*RFRCF(IS)+SUMW)
      LS(1,IC,IS)=(CCRITS(IC)*SCF(IC,IS)-CRB(IC)*RBCCF(IC,IS))/
     #  (A(1,1)*RFRCF(IS)+SUMS)
      LB(1,IC,IS)=(CCRITB(IC)*BCF(IC,IS)-CRB(IC)*RBCCF(IC,IS))/
     #  (A(1,1)*RFRCF(IS)+SUMB)
```

```
C
C  INITIALIZE OUTFALL LOOP, "IT"
C
      DO 300 IT=2,NOUTFL
      LW(IT,IC,IS)=(A(1,1)/A(IT,IT))*LW(1,IC,IS)
      LS(IT,IC,IS)=(A(1,1)/A(IT,IT))*LS(1,IC,IS)
      LB(IT,IC,IS)=(A(1,1)/A(IT,IT))*LB(1,IC,IS)
  300 CONTINUE
  200 CONTINUE
  100 CONTINUE
C
C  WRITE OUTPUT DATA
C
      DO 325 IC=1,NCHEM
      IOFILE=6+IC
      OPEN(IOFILE,FILE=OUTCHM(IC),STATUS='UNKNOWN')
      DO 350 IT=1,NOUTFL
      WRITE(IOFILE,605) IT
      DO 375 IS=1,NSI
      WRITE(IOFILE,610) LW(IT,IC,IS),LS(IT,IC,IS),LB(IT,IC,IS)
  375 CONTINUE
  350 CONTINUE
      CLOSE(IOFILE)
  325 CONTINUE
C
C  FORMAT STATEMENTS
C
  601 FORMAT(1X,'ENTER THE NAME OF THE OUTPUT FILE FOR CHEMICAL NO.',I3)
  605 FORMAT(1X,'---------------', 'OUTFALL NO. ',I5,'---------------')
  610 FORMAT(1X,3(E12.4,1X))
C
      STOP
      END
```

APPENDIX VIII

Source code listing of the MOEE-adaptation of the Thomann foodweb model

```
      PROGRAM FDWEB2
C
C***********************************************************************
C
C     PROGRAM FOR : "CHEMICAL FOODWEB MODEL WITH SEDIMENT INTERACTION"
C                    BY:  R.V. THOMANN OF MANHATTAN COLLEGE
C
C     PROGRAMMING BY:      Peter Nettleton,
C                          Ontario Ministry of the Environment
C
C                * * *  V E R S I O N   2.0  * * *
C
C     "Version 2" includes calibration factors for the Benthos'
C      Consumption of Sediment and Phytoplankton, (Eqs 12 & 11):
C      "CALSED" & "CALPHY"
C***********************************************************************
C
      DIMENSION A(5),AC(5),AOC(5),AWD(5),BAF(5),BETA(5),BSF(5),CBODY(5),
     #DEL(5),EC(5),FI(5),G(5,5),GAM(5),GROW(5),IL(5),K(5),KU(5),K1(5),
     #LIP(5),NW(5),RESP(5),W(5), ALF(5,5)
      CHARACTER FNAMEI*64,FNAMEO*64
      CHARACTER NAME(5)*17
      CHARACTER PHYTOPL DETRITUS*16
      CHARACTER ZOOPLANKTON*11
      CHARACTER FORAGE FISH*11
      CHARACTER PISCIVOROUS FISH*16
      CHARACTER BENTHIC INVERT*14
      REAL IL,ILOC5,K,KOW,KU,K1,LKOW,LIP,NW,MW
C
C     OPEN INPUT / OUTPUT FILES, VIA USER.
C
      WRITE(*,*) '****************************************************'
      WRITE(*,*) '  '
      WRITE(*,*) '  Enter the INPUT FILENAME : '
      WRITE(*,*) '  '
      READ(*,'(A)') FNAMEI
      WRITE(*,*) '  '
      WRITE(*,*) '****************************************************'
      WRITE(*,*) '  '
      WRITE(*,*) '  Enter the OUTPUT FILENAME : '
      WRITE(*,*) '  '
      READ(*,'(A)') FNAMEO
      WRITE(*,*) '  '
      WRITE(*,*) '****************************************************'
C
      OPEN(5,FILE=FNAMEI)
      OPEN(6,FILE=FNAMEO,STATUS='UNKNOWN')
C
      NAME(1)='PHYTO / DETRITUS'
      NAME(2)='ZOOPLANKTON'
      NAME(3)='FORAGE FISH'
      NAME(4)='PISCIVOROUS FISH'
      NAME(5)='BENTHIC INVERT'
C
C     READ / WRITE "ENVIRONMENTAL FACTORS":
C
      READ(5,*) CW,CS,RWD,RSD,FOCW,FOCS,LKOW,CO2,MW
      WRITE(6,601)
      WRITE(6,602) CW,CS,RWD,RSD,FOCW,FOCS,LKOW,CO2,MW
      KOW=10.0**LKOW
      RW=RWD/FOCW
      RS=RSD/FOCS
C
C     READ / WRITE "BIOTA-SPECIFIC PARAMETERS":
```

```
C
      NCOMP=5
      WRITE(6,603)
      DO 10 I=1,NCOMP
      READ(5,*) W(I),LIP(I),BETA(I),GAM(I),DEL(I),FI(I),A(I),AWD(I),
     #AOC(I),AC(I),K1(I)
      WRITE(6,604) I,W(I),LIP(I),BETA(I),GAM(I),DEL(I),FI(I),A(I),
     #AWD(I),AOC(I),AC(I),K1(I)
   10 CONTINUE
      READ(5,*) FOCB
      WRITE(6,612)FOCB
C
C     READ / WRITE "RESPIRATION & FEEDING OPTIONS" FOR
C     BENTHIC INVERTEBRATES & FORAGE FISH :
C
      READ(5,*) B5S,B5W
      READ(5,*) P5S,P51
      READ(5,*) P35,P32
      WRITE(6,605)
      WRITE(6,606) B5S,B5W
      WRITE(6,607) P5S,P51
      WRITE(6,608) P35,P32
C
C     READ / WRITE BENTHOS' CONSUMPTION EQUATIONS CALIBRATION FACTORS
C
      READ(5,*) CALSED,CALPHY
      WRITE(6,611) CALSED,CALPHY
C
      PCS=RS/CS
      PCWS=RS/CW
C
C     CALCULATE BIOTA-SPECIFIC PARAMETERS:
C
      DO 30 I=2,NCOMP
      IM=I-1
C     ASSIGN UPTAKE EFFICIENCY, "EC", USING "FIGURE 2":
      EC(I)=0.01
      IF(LKOW.GE.2.0.AND.LKOW.LE.4.0) EC(I)=10.0**(-2.6+0.5*LKOW)
      IF(LKOW.GT.4.0.AND.LKOW.LE.4.5) EC(I)=-4.15+1.10*LKOW
      IF(LKOW.GT.4.5.AND.LKOW.LE.6.5) EC(I)=0.80
      IF(LKOW.GT.6.5.AND.LKOW.LE.8.0) EC(I)=3.40-0.40*LKOW
      IF(LKOW.GT.8.0.AND.LKOW.LE.8.5) EC(I)=2.60-0.30*LKOW
      IF(LKOW.GT.8.5.AND.LKOW.LE.9.0) EC(I)=0.73-0.08*LKOW
C     ASSUME ASSIMILATION EFFICIENCY, "ALF", EQUALS "EC":
      ALF(I,IM)=EC(I)
      GROW(I)=DEL(I)/(W(I)**BETA(I))
      RESP(I)=FI(I)/(W(I)**GAM(I))
      KU(I)=((AOC(I)*AC(I)*RESP(I))/(AWD(I)*LIP(I)*CO2))*EC(I)
      K(I)=KU(I)/KOW + K1(I)
      NW(I)=KU(I)/(GROW(I) + K(I))
      IL(I)=((GROW(I) + RESP(I))/A(I))*(AWD(IM)/AWD(I))*LIP(IM)/LIP(I)
      G(I,IM)=ALF(I,IM)*IL(I)/(K(I) + GROW(I))
   30 CONTINUE
C     ASSIGN OR CORRECT VALUES FOR COMPARTMENTS 1, 3 & 5 :
      G(3,2)=G(3,2)*P32
      IL(5)=CALPHY*((GROW(5) + RESP(5))/A(5))*(AWD(1)/AWD(5))*(LIP(1)/LI
     #P(5))
      ILOC5=CALSED*((GROW(5) + RESP(5))/A(5))*(1./AWD(5))*(FOCB/LIP(5))
      ALF5S=EC(5)
      ALF51=EC(5)
      G5S=P5S*ALF5S*ILOC5/(K(5) + GROW(5))
      G(5,1)=P51*ALF51*IL(5)/(K(5) + GROW(5))
      ALF35=EC(3)
      G(3,5)=P35*ALF35*IL(3)/(K(3) + GROW(3))
```

```
      PCPRIM=PCS*PCWS/(B5S*PCWS + B5W*PCS)
C
C     LET THE PHYTOPLANKTON BCF, "NW(1)", EQUAL EQUATION 28.
C
      NW(1)=KOW/(1.+FOCW*KOW*MW/1.4)
C
C     CALCULATE THE "BIOTA SEDIMENT FACTOR" (BSF), FOR ALL BIOTA :
C
      BSF(5)=NW(5)/PCPRIM + G5S + G(5,1)*NW(1)/PCWS
      BSF(1)=NW(1)/PCWS
      BSF(2)=NW(2)/PCWS + G(2,1)*BSF(1)
      BSF(3)=NW(3)/PCWS + G(3,2)*BSF(2) + G(3,5)*BSF(5)
      BSF(4)=NW(4)/PCWS + G(4,3)*BSF(3)
C
C     CALCULATE THE "BIOACCUMULATION FACTOR" (BAF), AND THE
C     "WHOLE-BODY", CHEMICAL CONCENTRATION ; FOR ALL BIOTA.
C
      DO 40 I=1,NCOMP
      BAF(I)=PCWS*BSF(I)
      CBODY(I)=BAF(I)*CW*LIP(I)
   40 CONTINUE
C
C     WRITE RESULTS
C
      WRITE(6,609)
      DO 50 I=1,NCOMP
      WRITE(6,610) I,NAME(I),W(I),LIP(I),NW(I),BSF(I),BAF(I),CBODY(I)
   50 CONTINUE
C
C     FORMAT STATEMENTS
C
  601 FORMAT(/,'THOMANN: "CHEMICAL FOODWEB MODEL WITH SEDIMENT INTERACTI
     #ON"',//,'INPUT DATA USED FOR THIS SIMULATION:',/)
  602 FORMAT(/,'  a)  ENVIRONMENTAL FACTORS :',/,'  Cw = ',E10.3,' ug/L'
     #,/,'  Cs = ',E10.3,' ug/L',/,'  Rwd = ',E10.3,' ug/kgsed',/,'  Rsd
     # = ',E10.3,' ug/kgsed',/,'  Focw = ',F5.3,/,'  Focs = ',F5.3,/,
     #'  LKOW = ',F5.3,' log(L/kg)',/,'  cO2 = ',E10.3,' kg/L',/,
     #'  MW  = ',E10.3,' kg/L')
  603 FORMAT(/,'  b)  BIOTA SPECIFIC PARAMETERS :',/,'COMP No.',2X,
     #'W (gm)',4X,'LIP',3X,'BETA',2X,'GAM',3X,'DEL',4X,'FI',4X,'A',4X,
     #'AWD',3X,'AOC',4X,'AC',2X,'K1(1/d)',/)
  604 FORMAT(3X,I1,4X,F10.5,6(1X,F5.3),1X,F5.2,2(1X,F5.3),1X,F7.5)
  605 FORMAT(/,'  c)  RESPIRATION, FEEDING OPTION & CONSUMPTION CALIBRAT
     #ION PARAMETERS :',/)
  606 FORMAT('  FRACTION OF BENTHIC INVERTEBRATES "RESPIRATION VOLUME" F
     #ROM',/,'  SEDIMENT & WATER COLUMN, "B5S" & "B5W":',/,2X,2(F5.3,
     #5X))
  607 FORMAT('  FRACTION OF BENTHIC INVERTEBRATES "FOOD MASS" FROM',/,'
     # SEDIMENT & PHYTOPLANKTON / DETRITUS, "P5S" & "P51":',/,2X,2(F5.3,
     #5X))
  608 FORMAT('  FRACTION OF FORAGE FISH "FOOD MASS" FROM',/,'  BENTHIC I
     #NVERTEBRATES & ZOOPLANKTON, "P35" & "P32":',/,2X,2(F5.3,5X))
  609 FORMAT(/,'SIMULATION RESULTS',//,1X,'BIOTA COMPARTMENT:',6X,'W',
     #6X,'LIP',6X,'NW',9X,'BSF',8X,'BAF',5X,'BODY CONC',//,'No',5X,'NAME
     #',13X,'(G)',11X,'Lw/KGlip',2X,'KGoc/KGlip',2X,'Lw/KGlip',3X,
     #'UG/KGwet',/)
  610 FORMAT(/,I1,1X,A17,T21,F10.5,1X,F5.3,1X,4(E10.3,1X))
  611 FORMAT('  CALIBRATION FACTORS FOR BENTHOS CONSUMPTION EQUATIONS:',
     #/,'  "CALSED" = ',F6.3,3X,'  "CALPHY" = ',F6.3)
  612 FORMAT(8X,'BENTHIC INVERTEBRATE F.O.C. = ',F5.3)
      STOP
      END
```